Electronic Supplementary Material

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System Constant Database of an Extended Temperature Range for Open-Tubular Columns for Gas Chromatography

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Table S-1

Retention Factor Database for SPB-Octyl (60-260 °C)

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| compound | logk60 | logk80 | logk100 | logk120 | logk140 | logk160 | logk180 | logk200 | logk220 | logk240 | logk260 |
| 1-Acetonaphthone |  | 1.4706 | 1.3208 | 1.2472 | 0.9647 | 0.7237 | 0.5703 | 0.3012 | 0.1073 |  |  |
| 1-Bromododecane |  |  | 1.2290 | 0.9296 | 0.6683 | 0.5149 | 0.2179 | -0.0262 |  |  |  |
| 1-Bromonaphthalene |  |  | 1.1653 | 0.9022 | 0.6730 | 0.5195 | 0.2724 |  |  |  |  |
| 1-Chloronaphthalene |  |  | 0.9591 | 0.7092 | 0.4956 | 0.3422 | 0.1165 |  |  |  |  |
| 1-Hydroxyanthraquinone |  |  |  |  | 1.5479 | 1.4038 | 1.0222 | 0.7875 |  |  |  |
| 1-Naphthol |  |  | 1.0177 | 0.7639 | 0.5441 | 0.3907 | 0.1563 |  |  |  |  |
| 1-Nitronaphthalene |  |  | 1.2872 | 1.0110 | 0.7684 | 0.6149 | 0.3495 |  |  |  |  |
| 1-Nitropyrene |  |  |  |  |  | 2.1410 | 1.6526 | 1.3011 |  |  |  |
| 1,2-Dichlorobenzene |  |  | 0.1938 | 0.0080 | -0.1561 | -0.3095 | -0.4455 |  |  |  |  |
| 1,2-Dimethylbenzene |  |  | -0.1268 | -0.2944 | -0.4322 | -0.5856 | -0.6942 |  |  |  |  |
| 1,2,4,5-Tetrachlorobenzene | 1.3275 | 0.9790 | 0.6332 | 0.8724 | 0.6300 | 0.4156 | 0.2687 | 0.0339 | -0.1355 |  |  |
| 1,2,5,6-Dibenzoanthracene |  |  |  |  |  | 1.8051 | 1.6299 | 1.1846 | 0.9129 |  |  |
| 1,3-Dihydroxybenzene |  |  |  |  |  |  |  |  | -0.5277 |  |  |
| 1,3-Dimethylbenzene | 0.5353 | 0.2023 | -0.0937 | -0.3588 | -0.5961 | -0.1888 | -0.3536 | -0.4973 | -0.6507 | -0.7506 |  |
| 1,3-Dinitrobenzene |  |  |  |  |  | 0.8719 | 0.6241 | 0.4068 | 0.2534 | 0.0306 | -0.1453 |
| 1,3,5-Triethylbenzene |  |  |  |  |  | 0.5235 | 0.2875 | 0.0841 | -0.0694 | -0.2714 |  |
| 1,4-Dimethylbenzene | 0.5238 | 0.1923 | -0.1014 | -0.3623 | -0.5980 | -0.1888 | -0.3586 | -0.4881 | -0.6415 | -0.7244 |  |
| 1,12-dodecanediol |  |  |  |  | 1.3794 | 1.4319 | 1.1132 | 0.8334 | 0.6800 | 0.3601 | 0.1440 |
| 2-(1-naphthyl)ethanol |  |  |  |  | 1.2820 | 1.3866 | 1.0984 | 0.8426 | 0.6892 | 0.4081 | 0.2170 |
| 2-Acetonaphthone |  |  |  | 1.5476 | 1.1923 | 1.3172 | 1.0301 | 0.7860 | 0.6326 | 0.3538 | 0.1582 |
| 2-Chloroacetamide | 0.2391 | -0.0695 | -0.3909 | -0.6792 |  |  |  |  |  |  |  |
| 2-Chlorophenol |  |  |  |  |  |  |  |  |  |  | -0.6919 |
| 2-Methoxycinnamaldehyde |  |  |  | 1.2605 | 0.9056 | 1.0585 | 0.7870 | 0.5500 | 0.3909 |  | -0.0561 |
| 2-Methoxynaphthalene |  |  |  |  |  | 1.0299 | 0.7715 | 0.5448 | 0.3914 | 0.1451 | -0.0200 |
| 2-Methylaniline |  |  |  |  |  |  | -0.1696 | -0.3230 | -0.4633 |  |  |
| 2-Methylbenzothiazole |  |  |  |  |  |  |  | 0.2729 | 0.1273 | -0.0563 | -0.2367 |
| 2-Methylnaphthalene |  |  |  |  |  | 0.7726 | 0.5355 | 0.3305 | 0.1771 | -0.0314 |  |
| 2-Methylphenol |  |  |  |  |  | 0.0354 | -0.1461 | -0.2966 | -0.4500 | -0.5711 |  |
| 2-Naphthol |  |  |  |  |  | 1.0277 | 0.7699 | 0.5465 | 0.3931 | 0.1579 |  |
| 2-Nitroaniline |  |  |  |  |  | 0.7867 | 0.5526 | 0.3449 | 0.1915 | -0.0086 |  |
| 2-Nitrophenol |  |  |  |  |  | 0.3380 | 0.1426 | -0.0317 | -0.1851 | -0.3344 |  |
| 2-Phenylacetamide |  |  | 1.1707 | 0.8483 |  | 0.6875 | 0.4578 | 0.2333 | 0.0788 | -0.1042 | -0.2563 |
| 2-Phenylethanol |  |  |  |  |  | 0.2210 | 0.0188 | -0.1424 | -0.2958 | -0.4403 |  |
| 2-Undecanone |  |  |  |  |  | 0.5781 | 0.3346 | 0.1200 | -0.0334 | -0.2506 |  |
| 2,4-Dimethylaniline |  |  | 0.7719 | 0.4208 | 0.0897 |  |  |  |  |  |  |
| 2,4-Dinitroaniline |  |  |  |  |  |  | 1.3842 | 1.1072 | 0.9447 | 0.6389 | 0.4145 |
| 2,6-Dichloro-4-nitroaniline |  |  |  |  | 1.5052 | 1.4658 | 1.1737 | 0.9205 | 0.7712 | 0.4715 | 0.2727 |
| 3-Aminopropyltriethoxysilane |  | 1.2758 | 0.8431 | 0.4725 | 0.1328 | 0.3992 | 0.1606 | -0.0472 | -0.2006 | -0.4090 | -0.5959 |
| 3-Methylaniline |  |  |  |  |  | 0.1755 | -0.0158 | -0.1763 | -0.3297 | -0.4720 |  |
| 3-Methylphenol |  |  |  |  |  | 0.0524 | -0.1294 | -0.2849 | -0.4384 | -0.5725 |  |
| 3-Nitroaniline |  |  |  |  |  | 0.8758 | 0.6362 | 0.4203 | 0.2669 | 0.0442 |  |
| 3,3'-Dichlorobenzidine |  |  |  |  |  |  |  | 2.0290 | 1.6930 | 1.4090 | 1.1430 |
| 3,4-Dichloroanilne |  |  |  |  |  | 0.8677 | 0.6259 | 0.4113 | 0.2579 | 0.0438 |  |
| 3,5-Dimethylphenol |  |  |  |  |  | 0.2891 | 0.0855 | -0.0872 | -0.2406 | -0.4109 |  |
| 4-acetylbiphenyl |  |  |  |  |  | 1.6934 | 1.3784 | 1.0966 | 0.9431 | 0.6084 |  |
| 4-Bromoacetanilide |  |  |  |  |  | 1.2511 | 0.9290 | 0.7703 | 0.6078 |  |  |
| 4-Chloroaniline |  |  |  |  |  | 0.4084 | 0.2185 | 0.0402 | -0.1132 | -0.2666 |  |
| 4-Chloro-2-nitroaniline |  |  |  |  |  | 1.1822 | 0.8917 | 0.6586 | 0.5061 | 0.2658 |  |
| 4-Chlorophenol |  |  |  |  |  | 0.2720 | 0.0698 | -0.0987 | -0.2521 | -0.4024 |  |
| 4-Dimethylaminoazobenzene |  |  |  |  |  |  |  | 1.4381 | 1.2820 | 0.9087 | 0.6692 |
| 4-Fluoroaniline | 0.7360 | 0.3871 | 0.0807 | -0.1893 | -0.4299 | -0.0582 | -0.2333 | -0.3838 | -0.5258 | -0.6881 | -0.7872 |
| 4-Hydroxybenzaldehyde |  |  |  |  |  | 0.5214 | 0.2898 | 0.1097 | -0.0437 | -0.1814 |  |
| 4-Hydroxybezyl alcohol |  |  |  |  |  | 0.5076 | 0.2879 | 0.1027 | -0.0507 | -0.2351 |  |
| 4-Methoxybenzyl alcohol |  |  | 0.9212 | 0.5810 | 0.2801 | 0.5442 | 0.3143 | 0.1193 | -0.0324 | -0.2287 | -0.3887 |
| 4-Methoxy-2-nitroaniline |  |  |  |  |  |  | 1.0190 | 0.6902 | 0.5312 | 0.2819 |  |
| 4-Methylphenol |  |  |  |  |  | 0.0438 | -0.1334 | -0.2878 | -0.4412 |  |  |
| 4-Nitroaniline |  |  |  |  |  | 1.0708 | 0.8106 | 0.5834 | 0.4300 | 0.1921 |  |
| 4-Nitrotoluene |  |  |  |  |  | 0.4832 | 0.2795 | 0.0938 | -0.0596 | -0.2383 |  |
| 4-Phenylphenol |  |  |  |  |  | 1.3921 | 1.0937 | 0.8364 | 0.6830 | 0.3948 |  |
| 4,4'-Dibromobiphenyl |  |  |  |  |  |  |  | 1.4638 | 1.3135 | 0.9415 | 0.7052 |
| 4,4'-Methylenedianiline |  |  |  |  |  |  |  | 1.4845 | 1.3106 | 0.9508 | 0.7015 |
| 8-Hydroxyquinoline |  |  |  |  |  |  |  | 0.3723 | 0.2301 | 0.0334 | -0.1335 |
| Acenaphthene |  |  |  |  |  |  |  |  |  |  | 0.0725 |
| Acenaphthylene |  |  |  |  |  | 1.0863 | 0.8947 | 0.6055 | 0.4521 | 0.2141 | 0.0301 |
| Acetamide | -0.3019 | -0.6237 | -0.8396 |  | -1.1150 |  |  |  |  |  |  |
| Acetoacetanilide |  |  | 0.6964 | 0.3687 | 0.0730 |  |  |  |  |  |  |
| Acetophenone |  |  |  |  |  | 0.1640 | -0.0302 | -0.1916 | -0.3450 | -0.4842 |  |
| Amyl cinnamal |  |  |  |  | 1.2399 | 1.3314 | 1.0335 | 0.7707 | 0.6645 | 0.3200 | 0.1097 |
| Androsterone |  |  |  |  |  |  |  |  | 2.0043 |  |  |
| Aniline |  |  |  |  |  | -0.0542 | -0.2253 | -0.3703 | -0.5238 | -0.6426 |  |
| Anisole |  |  |  |  |  | -0.1383 | -0.3062 | -0.4582 | -0.6116 | -0.7090 |  |
| Anthracene |  |  |  |  |  |  | 1.4358 | 1.1638 | 1.0104 | 0.6896 | 0.4786 |
| Anthraquinone |  |  |  |  |  |  |  | 1.4013 | 1.2546 | 0.8930 | 0.6524 |
| Azulene |  |  |  |  |  |  |  | 0.3433 |  | 0.0069 | -0.1608 |
| Benzaldehyde |  |  |  |  |  | -0.0563 | -0.2235 | -0.3669 | -0.5203 | -0.6330 |  |
| Benz[a]anthracene |  |  |  |  |  |  |  | 2.1327 | 1.9900 | 1.5183 | 1.2504 |
| Benzamide |  |  |  |  |  | 0.5605 | 0.3366 | 0.1558 | 0.0023 | -0.1854 |  |
| Benzidine |  |  |  |  |  |  |  | 1.4656 |  | 0.9374 | 0.7009 |
| Benz[a]pyrene |  |  |  |  |  |  |  |  |  | 1.9957 | 1.7030 |
| Benzenesulfonamide |  |  |  |  |  | 0.8912 | 0.6420 | 0.4298 | 0.2764 | 0.0491 | -0.1026 |
| Benzophenone |  |  |  |  |  | 1.3227 | 1.0368 | 0.7828 | 0.6294 | 0.3442 |  |
| Benzo[e]pyrene |  |  |  |  |  |  |  |  |  | 1.9810 | 1.6896 |
| Benzo[ghi]perylene |  |  |  |  |  |  |  |  |  | 2.4841 | 2.1828 |
| Benzyl alcohol |  |  |  |  |  | 0.0299 | -0.1425 | -0.2907 | -0.4441 | -0.5711 |  |
| Benzothiazole |  |  |  |  |  |  |  | 0.1558 | 0.0092 | -0.1450 | -0.3161 |
| Benzyl cinnamate |  |  |  |  |  |  | 1.8200 | 1.4953 | 1.3036 | 0.9466 | 0.6796 |
| Benzyl 2-ethylhexyl phthalate |  |  |  |  |  |  |  |  | 1.9202 | 1.4398 |  |
| Benzyl salicylate |  |  |  |  |  | 1.7930 | 1.4622 | 1.1717 | 1.0079 | 0.6762 | 0.4389 |
| Borneol |  |  | 0.7146 | 0.4024 | 0.1256 | 0.4263 | 0.2213 | 0.0406 | -0.0995 | -0.2770 | -0.4227 |
| Butyl benzyl phthalate |  |  |  |  |  |  |  | 1.8094 | 1.6260 | 1.1820 | 0.9077 |
| Butyl cyclohexyl phthalate |  |  |  |  |  |  |  |  | 1.5051 | 1.0385 | 0.7738 |
| Butyl decyl phthalate |  |  |  |  |  |  | 1.5024 | 1.1915 | 1.0085 | 0.6600 | 0.4104 |
| Butyl octyl phthalate |  |  |  |  |  |  | 1.5056 | 1.1914 | 1.0380 | 0.6488 | 0.4087 |
| Butyl oleate |  |  |  |  |  |  |  | 1.9114 | 1.5909 | 1.2495 | 0.9319 |
| Butyl stearate |  |  |  |  |  |  |  |  | 1.6344 | 1.2899 | 0.9674 |
| Carbazole |  |  |  |  |  |  | 1.3855 | 1.1143 | 0.9609 | 0.6484 | 0.4401 |
| Camphor |  |  | 0.6313 | 0.3223 | 0.0530 | 0.3673 | 0.1654 | -0.0096 | -0.1463 | -0.3256 | -0.4700 |
| Carvone |  |  | 1.2008 | 0.8472 | 0.5165 | 0.5361 | 0.3110 | 0.1154 | -0.0351 | -0.2339 | -0.3600 |
| Chrysene |  |  |  |  |  |  |  |  |  | 1.5445 | 1.2570 |
| Cinnamyl alcohol |  |  |  |  |  | 0.6128 | 0.3837 | 0.1854 | 0.0320 | -0.1666 |  |
| Citronellal |  |  | 0.6007 | 0.2716 | -0.0201 | 0.2856 | 0.0687 | -0.1130 | -0.2677 | -0.4427 | -0.4960 |
| Coumarin |  |  |  |  |  | 0.9038 | 0.6544 | 0.4505 | 0.2971 | 0.0766 | -0.0970 |
| Cyclohexanone oxime |  | 0.5998 | -0.1038 | -0.2498 |  | 0.0840 | -0.1038 | -0.2498 | -0.4032 | -0.5304 |  |
| Decan-1-ol |  |  |  |  |  | 0.5224 | 0.2616 | 0.0732 | -0.0802 | -0.2862 |  |
| Decane |  |  |  |  |  | 0.0408 | -0.1630 | -0.3295 | -0.4829 | -0.6346 |  |
| Dibenzofuran |  |  |  |  |  | 1.2049 | 0.9356 | 0.6999 | 0.5465 | 0.2887 |  |
| Dibenzylamine |  |  |  |  |  |  | 1.2280 | 0.9574 | 0.8040 | 0.4890 |  |
| Dibenzyl ether |  |  |  |  | 1.2930 | 1.3872 | 1.0902 | 0.8271 | 0.6737 | 0.3739 | 0.1701 |
| Di(2-n-butoxyethyl) phthalate |  |  |  |  |  |  |  | 1.9657 | 1.7655 | 1.3080 | 0.9911 |
| Di-n-Butyl phthalate |  |  |  |  |  |  | 1.5037 | 1.1937 | 1.0103 | 0.6624 | 0.4116 |
| Di-n-Butyl succinate |  |  |  |  |  |  | 0.7464 | 0.4933 | 0.3137 | 0.0533 | -0.1503 |
| Dicyclohexyl phthalate |  |  |  |  |  |  |  |  | 1.8976 | 1.4436 | 1.1332 |
| Dicyclohexylamine |  |  |  | 1.2823 | 0.9203 | 0.9970 | 0.7399 | 0.5039 | 0.3393 | 0.1070 | -0.0801 |
| Dicylcohexyl adipate |  |  |  |  |  |  |  |  |  | 1.1328 |  |
| Di(2-Ethoxyethyl) phthalate |  |  |  |  |  |  | 1.7155 | 1.3809 | 1.1907 | 0.8148 | 0.5443 |
| Di-2-ethylhexyl phthalate |  |  |  |  |  |  |  |  | 1.9202 | 1.4400 | 1.0578 |
| Diethyl adipate |  |  |  |  |  |  | 0.3876 | 0.1647 | -0.0075 | -0.2287 | -0.4111 |
| N,N-Diethylcarbanilide |  |  |  |  |  | 1.7427 | 1.4186 | 1.1336 | 0.9714 | 0.6429 | 0.4132 |
| Diethyl diethylmalonate |  |  |  |  |  |  | 0.2173 | 0.0150 | -0.1526 | -0.3560 | -0.5100 |
| N,N-Diethyldodecamide |  |  |  |  |  | 1.8948 | 1.5286 | 1.2060 | 1.0198 | 0.6590 | 0.4097 |
| N,N-Diethyl-4-nitroaniline |  |  |  |  |  |  | 1.4075 | 1.1375 | 0.9695 | 0.6509 | 0.4195 |
| Diethyl phthalate |  |  |  | 1.3661 | 0.9923 | 1.1202 | 0.8347 | 0.5852 | 0.4173 | 0.1537 | -0.0495 |
| Diethyl sebecate |  |  |  |  |  |  | 1.1598 | 0.8669 | 0.6769 | 0.3855 | 0.1304 |
| Diisobutyl phalate |  |  |  |  |  |  | 1.3375 | 1.0375 | 0.8841 | 0.5227 | 0.2954 |
| Di-(2-Methoxyethyl) phthalate |  |  |  |  |  |  | 1.4977 | 1.1865 | 1.0041 | 0.6584 | 0.4061 |
| N,N-Dimethylaniline | 1.2768 | 0.9145 |  |  | -0.0422 |  |  |  |  |  |  |
| N,N-Dimethyl-4-nitroaniline |  |  |  |  |  | 1.4746 | 1.1439 | 0.8542 | 0.7395 |  |  |
| Dimethyl phthalate |  |  |  |  |  |  | 0.5747 | 0.3473 | 0.1895 | -0.0381 | -0.2177 |
| Di-n-Octyl phthalate |  |  |  |  |  |  |  |  |  |  | 1.3439 |
| Diphenylamine |  |  |  |  |  | 1.3121 | 1.0227 | 0.7783 | 0.6240 | 0.3370 |  |
| Diphenyl ether |  |  |  | 1.2489 | 0.8842 | 0.9052 | 0.6537 | 0.4320 | 0.2786 | 0.0442 |  |
| N,N-Diphenyl-4-phenylenediamine |  |  |  |  |  |  |  |  |  | 1.6777 | 1.3637 |
| Dodecamethylcyclohexasiloxane |  |  |  |  |  | 0.4592 | 0.2017 | -0.0222 | -0.1756 | -0.4061 |  |
| Dodecane |  |  |  |  |  | 0.4693 | 0.2326 | 0.0246 | -0.1288 | -0.3312 |  |
| Ethyl oleate |  |  |  |  |  |  | 1.9537 | 1.5908 | 1.2965 | 0.9786 | 0.6852 |
| Eugenol |  |  | 1.1887 | 0.8270 | 0.5035 | 0.7225 | 0.4757 | 0.2659 | 0.1090 | -0.1090 | -0.2870 |
| Fluoranthene |  |  |  |  |  |  |  | 1.5772 | 1.4238 | 1.0464 | 0.8080 |
| Fluorene |  |  |  |  |  | 1.3437 | 1.0629 | 0.8172 | 0.6638 | 0.3924 | 0.1921 |
| Geranial |  |  |  |  |  | 0.5220 | 0.2882 | 0.1761 | -0.0732 | -0.2737 |  |
| Geraniol |  |  | 0.8583 | 0.5079 | 0.1982 | 0.4636 | 0.2348 | 0.0358 | -0.1239 | -0.3165 | -0.4834 |
| Glycidoxypropyltrimethoxysilane |  |  | 1.3226 | 0.9169 | 0.5504 | 0.7721 | 0.5025 | 0.2684 | 0.1149 | -0.1363 | -0.3363 |
| Hexachlorobenzene |  |  |  |  |  | 1.6389 | 1.3433 | 1.0752 | 0.9218 | 0.6106 | 0.3981 |
| Hexadecane |  |  |  |  |  | 1.3277 | 1.0030 | 0.7238 | 0.5704 | 0.2450 |  |
| Hydroxycitronellal |  |  |  |  |  | 0.5092 | 0.2763 | 0.0778 | -0.0820 | -0.2778 | -0.3160 |
| Iodobenzene |  |  |  |  |  | 0.2465 | 0.0697 | -0.1001 | -0.2535 | -0.4052 |  |
| alpha-Isomethyl ionone |  |  | 1.5682 | 1.1319 | 0.8331 | 0.9985 | 0.7301 | 0.4977 | 0.3383 | 0.0944 | -0.0998 |
| Isocyanatopropyltriethoxysilane |  |  | 1.0999 | 0.7091 | 0.3516 | 0.5940 | 0.3365 | 0.1085 | -0.0449 | -0.2763 | -0.4740 |
| Lilial |  |  |  | 1.3141 | 0.9570 | 1.0969 | 0.8227 | 0.5813 | 0.4216 | 0.1629 | -0.0334 |
| Limonene |  |  | 0.3931 | 0.0885 | -0.1786 | 0.1603 | -0.0343 | -0.1989 | -0.3524 | -0.5057 | -0.6442 |
| Linalool |  |  | 0.4566 | 0.1363 | -0.1452 | 0.1790 | -0.0244 | -0.2003 | -0.3470 | -0.5154 | -0.6811 |
| Methacryloxypropyltrimethoxysilane | |  | 1.2910 | 0.8816 | 0.5106 | 0.7311 | 0.4568 | 0.2202 | 0.0668 | -0.1894 | -0.3931 |
| Methyl abietate |  |  |  |  |  |  |  | 1.9061 | 1.6066 | 1.3017 | 1.0056 |
| N-Methylacetamide | 0.0388 | -0.2429 | -0.5501 | -0.8491 | -0.9735 |  |  |  |  |  |  |
| Methyl eugenol |  |  | 1.6649 | 1.2506 | 0.8591 | 0.8017 | 0.5400 | 0.3139 | 0.1486 | -0.0818 | -0.2651 |
| Methyl nonanoate |  | 1.2140 | 0.8072 | 0.4524 | 0.1411 |  | 0.1776 | -0.0366 | -0.1953 | -0.4015 | -0.5445 |
| Naphthalene |  |  |  |  |  | 0.5483 | 0.3279 | 0.1487 | -0.0047 | -0.1820 |  |
| Neral |  |  | 1.1593 | 0.7994 | 0.4622 | 0.4661 | 0.2390 | 0.0868 | -0.0732 | -0.2737 |  |
| Nicotinamide |  |  | 1.0853 | 0.7115 | 0.3853 | 0.6292 | 0.3982 | 0.2041 | 0.0578 | -0.1581 | -0.3019 |
| Nicotine |  |  |  | 0.8668 | 0.5532 | 0.7764 | 0.5381 | 0.3296 | 0.1840 | -0.0449 | -0.1990 |
| Nonane |  |  |  |  |  | -0.1798 | -0.3723 | -0.5152 | -0.6687 | -0.7852 |  |
| Octadecane |  |  |  |  |  |  | 1.3852 | 1.0683 | 0.9149 | 0.5256 |  |
| Octaethylcyclotetrasiloxane |  |  |  |  |  | 1.4647 | 1.1319 | 0.8384 |  | 0.3354 |  |
| n-Octyltriethoxysilane |  |  |  | 1.2916 | 0.7698 | 0.9384 | 0.6496 |  |  |  | -0.2896 |
| Octan-1-ol | 1.1072 | 0.7008 | 0.3482 | 0.0411 | -0.2300 |  |  |  |  |  | -0.8272 |
| Octanophenone |  |  |  |  |  | 1.4038 | 1.0936 | 0.8221 | 0.6687 |  | 0.1379 |
| Pentachlorophenol |  |  |  |  |  | 1.6202 | 1.3161 | 1.0494 | 0.8960 | 0.5843 |  |
| Phenanthrene |  |  |  |  |  |  | 1.4194 | 1.1493 | 0.9959 | 0.6786 | 0.4626 |
| Phenol |  |  |  |  |  | -0.1837 | -0.3421 | -0.4779 | -0.6313 | -0.7264 |  |
| Phenyl acetate |  |  |  |  |  | 0.0754 | -0.1047 | -0.2835 | -0.4369 | -0.5562 |  |
| Phenylcyclohexane |  |  |  | 0.8937 | 0.5810 | 0.8075 | 0.5688 | 0.3544 | 0.2010 | -0.0105 |  |
| Phthalimide |  |  |  |  |  | 0.8506 | 0.6025 | 0.3969 | 0.2435 | 0.0265 |  |
| Phthalonitrile |  |  |  |  |  | 0.5187 | 0.3093 | 0.1146 | -0.0388 | -0.2069 |  |
| alpha-Pinene |  |  | 0.1139 | -0.1684 | -0.4114 | -0.0275 | -0.2079 | -0.3518 | -0.4954 | -0.6294 | -0.7844 |
| beta-Pinene |  |  | 0.2537 | -0.0329 | -0.1629 | 0.0841 | -0.1021 | -0.2524 | -0.3942 | -0.6294 | -0.6919 |
| Quinine |  |  |  |  |  |  |  |  |  | 1.8540 | 1.5672 |
| Quinoline |  |  |  |  |  | 0.6079 | 0.3893 | 0.1984 | 0.0449 | -0.1338 | -0.3001 |
| Trans Stilbene |  |  |  |  |  | 1.5484 | 1.2397 | 0.9685 | 0.8151 | 0.5006 | 0.2884 |
| Styrene | 0.5893 | 0.2555 | -0.0519 | -0.3018 | -0.5565 | -0.1463 | -0.3154 | -0.4580 | -0.6041 | -0.7608 | -0.8750 |
| p-Terphenyl |  |  |  |  |  |  |  | 1.7158 | 1.5567 | 1.1385 | 0.8820 |
| Terpinen-4-ol |  |  | 0.7855 | 0.4563 | 0.1680 | 0.4525 | 0.2363 | 0.0512 | -0.0995 | -0.2844 | -0.4408 |
| Thioacetamide | 0.6306 | 0.2897 | -0.0553 | -0.2393 | -0.3470 |  |  |  |  |  |  |
| Tribenzylamine |  |  |  |  |  |  |  | 1.8364 | 1.6628 | 1.2342 | 0.9536 |
| Tri-n-Butyrin |  |  |  |  |  |  |  | 0.9082 | 0.7548 | 0.3832 | 0.1541 |
| Triethylamine | -0.2213 | -0.5140 | -0.7873 |  |  |  |  |  |  |  |  |
| Triisopropanolamine |  |  | 1.3133 | 0.9152 | 0.5624 |  | 0.5051 | 0.2908 | 0.1282 | -0.0962 | -0.2676 |
| Trimethoprin |  |  |  |  |  |  |  |  | 1.9174 | 1.4604 | 1.1576 |
| Triphenylene |  |  |  |  |  |  |  | 2.0967 | 1.8972 | 1.5310 | 1.2633 |
| Triphenylmethane |  |  |  |  |  |  |  | 1.3943 | 1.2409 | 0.8590 | 0.6185 |
| Undecane |  |  |  |  |  | 0.2568 | 0.0354 | -0.0982 | -0.2516 | -0.4831 |  |
| Valerophenone |  |  |  |  |  | 0.7704 | 0.5200 | 0.3044 | 0.1510 | -0.0725 | -0.2536 |
| Vanillin |  |  | 1.2108 | 0.8565 | 0.5380 | 0.7592 | 0.5153 | 0.3099 | 0.1570 | -0.0634 | -0.2304 |

Table S-2

Retention factor database for HP-5 (60 – 300 °C)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| compound | log60 | log80 | log100 | log120 | log140 | log160 | log180 | log200 | log220 | log240 | log260 | log280 | log300 |
| 1-Acetonaphthone |  |  | 2.1900 | 1.8305 | 1.4719 | 0.4662 | 0.1885 | -0.0574 | -0.2838 | -0.4752 | -0.6208 | -0.7791 | -0.8882 |
| 1-Bromododecane |  |  |  |  |  | 0.3919 | 0.0991 | -0.1576 | -0.3875 | -0.5867 | -1.0040 | -1.2060 | -1.2820 |
| 1-Bromonaphthalene |  |  |  |  |  | 0.2938 | 0.0397 | -0.1861 | -0.3891 | -0.5676 |  |  |  |
| 1-Chloronaphthalene |  |  |  |  |  | 0.1101 | -0.1307 | -0.3444 | -0.5360 | -0.7041 |  |  |  |
| 1-Hexyne | 0.0824 | -0.1750 | -0.3920 | -0.5850 | -0.7560 |  |  |  |  |  |  |  |  |
| 1-Hydroxyanthraquinone |  |  |  |  |  |  |  | 0.7441 | 0.4725 | 0.2274 | 0.0074 | -0.1906 | -0.3495 |
| 1-Naphthol |  |  |  |  |  | 0.3192 | 0.0492 | -0.1876 | -0.4034 | -0.5833 |  |  |  |
| 1-Nitronaphthalene |  |  |  |  |  | 0.5170 | 0.2391 | -0.0058 | -0.2289 | -0.4213 |  |  |  |
| 1-Nitropyrene |  |  |  |  |  |  |  | 1.4560 | 1.0070 | 0.7851 | 0.5652 | 0.3350 | 0.1126 |
| 1,12-dodecanediol |  |  |  | 2.2607 | 1.8247 | 0.7644 | 0.4305 | 0.1386 | -0.1219 | -0.3519 | -0.5588 |  | -0.8015 |
| 1,2-Dichlorobenzene |  | 1.1740 | 0.8835 | 0.5732 | 0.3281 | -0.5721 | -0.7563 | -0.9177 |  |  |  |  |  |
| 1,2-Dimethylbenzene | 1.0683 | 0.7370 | 0.4218 | 0.2025 | -0.0160 | -0.8804 |  |  |  |  |  |  |  |
| 1,2,4,5-Tetrachlorobenzene |  | 2.0309 | 1.5768 | 1.2622 | 0.9622 | 0.0038 | -0.2332 | -0.4407 | -0.6334 | -0.7816 | -0.9576 | -1.0891 | -1.1729 |
| 1,2,4-Trichlorobenzene |  |  |  | 0.9171 | 0.6409 |  |  |  |  |  |  |  |  |
| 1,3-Dichlorobenzene |  | 1.0830 | 0.7697 | 0.4955 | 0.2556 |  |  |  |  |  |  |  |  |
| 1,3-Dihydroxybenzene |  |  |  |  |  | -0.1871 | -0.4077 | -0.6364 | -0.8109 | -0.9822 | -1.1020 |  |  |
| 1,3-Dimethylbenzene | 0.9865 | 0.6610 | 0.3797 | 0.1338 | -0.0800 | -0.9485 |  |  |  |  |  |  |  |
| 1,3-Dinitrobenzene |  |  |  |  |  | 0.2161 | -0.0455 | -0.2746 | -0.4823 | -0.6551 | -0.7889 | -0.9379 | -1.0479 |
| 1,3,5-Triethylbenzene |  |  |  |  |  | -0.2576 | -0.4904 | -0.6932 | -0.8701 |  |  |  |  |
| 1,4-Dimethylbenzene | 0.9880 | 0.6620 | 0.3812 | 0.1355 | -0.0780 |  |  |  |  |  |  |  |  |
| 1,3-bis(trimethylsiloxy)-1,3-dimethylsilane | 1.4637 | 1.0136 | 0.6784 | 0.3643 | 0.0330 |  |  |  |  |  |  |  |  |
| 1,5-Dichloro-1,1,3,3,5,5-hexamethyltrisiloxane | 1.6046 | 1.1581 | 0.8207 | 0.5048 | 0.2109 |  |  |  |  |  |  |  |  |
| 1,5-Divinyl-1,1,3,3,5,5-hexamethyltrsiloxanane | 1.6267 | 1.1757 | 0.8323 | 0.5110 | 0.2363 |  |  |  |  |  |  |  |  |
| 2-(1-naphthyl)ethanol |  |  |  | 2.0172 | 1.6400 |  |  | 0.0736 | -0.1504 | -0.3519 | -0.5317 | -0.7237 | -0.8083 |
| 2-Acetonaphthone |  |  |  | 1.8909 | 1.5298 | 0.5270 | 0.2446 | -0.0052 | -0.2377 | -0.4273 | -0.5915 | -0.7942 | -0.8678 |
| 2-Chloroacetamide | 0.9631 | 0.7065 | 0.4130 | 0.1414 | -0.1499 |  |  |  |  |  |  |  |  |
| 2-Chloroaniline |  |  | 1.1007 | 0.7923 | 0.5238 |  |  |  |  |  |  |  |  |
| 2-Ethoxyethanol | 0.4242 | 0.1380 | -0.1059 | -0.3190 | -0.5020 |  |  |  |  |  |  |  |  |
| 2-Hexanone | 0.6946 | 0.3830 | 0.1153 | -0.1180 | -0.3190 |  |  |  |  |  |  |  |  |
| 2-Methoxycinnamaldehyde |  |  | 2.0965 | 1.7272 | 1.3656 | 0.3649 | 0.0823 | -0.1627 | -0.3803 | -0.5741 | -0.7950 |  |  |
| 2-Methoxyethanol | 0.1434 | -0.1180 | -0.3370 | -0.5270 | -0.6910 |  |  |  |  |  |  |  |  |
| 2-Methoxynaphthalene |  |  |  |  |  | 0.2289 | -0.0315 | -0.2564 | -0.4605 | -0.6409 |  |  |  |
| 2-Methylbutan-1-ol | 0.5146 | 0.2140 | -0.0412 | -0.2620 | -0.4550 |  |  |  |  |  |  |  |  |
| 2-Methyl-2-butanol | 0.1578 | -0.1070 | -0.3318 | -0.5270 | -0.6910 |  |  |  |  |  |  |  |  |
| 2-Methylaniline |  |  |  |  |  | -0.5258 | -0.7196 | -0.8945 | -1.0427 | -1.1829 |  |  |  |
| 2-Methylbenzothiazole |  |  |  |  |  |  |  | -0.4190 | -0.6412 | -0.8154 | -0.9745 | -1.0849 | -1.1841 |
| 2-Methylbutanol | 0.5146 | 0.2140 | -0.0412 | -0.2620 | -0.4550 |  |  |  |  |  |  |  |  |
| 2-Methylnaphthalene |  |  |  |  |  | -0.0591 | -0.2922 | -0.5032 | -0.6808 | -0.8467 |  |  |  |
| 2-Methylphenol |  |  |  |  |  | -0.6095 | -0.8066 |  |  |  |  |  |  |
| 2-Methylpropanol | 0.1030 | -0.1620 | -0.3862 | -0.5760 | -0.7440 |  |  |  |  |  |  |  |  |
| 2-Naphthol |  |  |  |  |  | 0.3336 | 0.0633 | -0.1735 | -0.3809 | -0.5606 |  |  |  |
| 2-Nitroaniline |  |  |  |  |  | 0.1393 | -0.1150 | -0.3257 | -0.5349 | -0.7041 |  |  |  |
| 2-Nitrophenol |  |  |  |  |  | -0.3812 | -0.5814 | -0.7534 | -0.9231 | -1.0531 |  |  |  |
| 2-Nitrotoluene |  |  |  |  |  | -0.2454 | -0.4798 | -0.6645 | -0.8835 | -1.0103 | -1.1708 |  |  |
| 2-Pentanone | 0.3259 | 0.0490 | -0.1875 | -0.3940 | -0.5760 |  |  |  |  |  |  |  |  |
| 2-Phenylacetamide |  |  |  | 1.2499 | 1.0520 | 0.0698 | -0.1334 | -0.3053 | -0.5298 | -0.6862 | -0.8327 |  |  |
| 2-Phenylethanol |  |  |  |  |  | -0.4584 | -0.6515 |  |  |  |  |  |  |
| 2-Undecanone |  |  |  |  |  | -0.1411 | -0.3816 | -0.5998 | -0.7961 | -0.9504 |  |  |  |
| 2,4-Dimethylaniline |  |  |  |  |  |  | -0.4976 |  |  |  |  |  |  |
| 2,4-Dinitroaniline |  |  |  |  |  |  | 0.7829 | 0.4790 |  |  | -0.1231 |  |  |
| 2,6-Dichloro-4-nitroaniline |  |  |  |  |  | 0.7218 | 0.4214 | 0.1480 | -0.0747 | -0.2919 | -0.4791 | -0.6723 | -0.7530 |
| 2,6-Dimethylphenol |  |  | 1.0264 | 0.7175 | 0.4490 |  |  |  |  |  |  |  |  |
| 2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane |  |  |  | 1.1410 | 0.8098 |  |  |  |  |  |  |  |  |
| 3-Aminopropyltriethoxysilane | 2.4214 | 1.8936 | 1.4702 | 1.0771 | 0.7456 |  |  |  |  |  |  |  |  |
| 3-Methylaniline |  |  |  |  |  | -0.5215 | -0.7146 | -0.8945 | -1.0534 | -1.1878 |  |  |  |
| 3-Methylbutanol | 0.5095 | 0.2060 | -0.0451 | -0.2770 | -0.4650 |  |  |  |  |  |  |  |  |
| 3-Methylphenol |  |  |  |  |  | -0.5793 | -0.7750 |  |  |  |  |  |  |
| 3-Nitroaniline |  |  |  |  |  | 0.2852 | 0.0200 | -0.2167 | -0.4267 | -0.6085 |  |  |  |
| 3-Nitrotoluene |  |  |  |  |  | -0.1840 | -0.4044 | -0.5922 | -0.8174 | -0.9714 |  |  |  |
| 3,3'-Dichlorobenzidine |  |  |  |  |  |  |  | 1.2798 | 0.9476 | 0.6522 | 0.3941 | 0.1656 | -0.0526 |
| 3,4-Dichloroanilne |  |  |  |  |  | 0.1825 | -0.0730 | -0.2963 | -0.4961 | -0.6714 |  |  |  |
| 3,5-Dimethylphenol |  |  |  |  |  | -0.3819 | -0.5976 | -0.7843 | -0.9507 | -1.0830 |  |  |  |
| 4-acetylbiphenyl |  |  |  | 2.3514 | 1.9397 | 0.9037 | 0.5813 | 0.2967 | 0.0374 | -0.1843 |  |  |  |
| 4-Bromoacetanilide |  |  |  |  |  |  | 0.4415 | 0.1005 | -0.0680 |  | -0.4293 |  |  |
| 4-Chloroaniline |  |  |  |  |  | -0.2570 | -0.4720 | -0.6642 | -0.8448 | -0.9800 |  |  |  |
| 4-Chlorophenol |  |  |  |  |  | -0.3250 | -0.5474 | -0.7329 |  |  |  |  |  |
| 4-Cyanophenol |  | 2.1937 |  |  | 1.0933 | 0.0954 | -0.1751 | -0.4096 | -0.6078 | -0.7671 |  |  |  |
| 4-Dimethylaminoazobenzene |  |  |  |  |  |  |  |  | 0.4489 | 0.1973 | -0.0314 | -0.2343 | -0.4071 |
| 4-Fluoroaniline | 1.4931 | 1.0751 | 0.7362 | 0.4596 | 0.2136 | -0.6905 | -0.8838 | -1.0420 |  | -1.3035 |  |  |  |
| 4-Hydroxybenzaldehyde |  |  |  |  |  | -0.0029 | -0.2573 | -0.4774 | -0.6777 | -0.8018 |  |  |  |
| 4-Hydroxybezylalcohol |  |  |  |  |  | -0.0384 | -0.2810 | -0.4862 | -0.6808 | -0.8490 |  |  |  |
| 4-Methoxy-2-nitroaniline |  |  |  |  |  |  | 0.2659 | 0.0307 | -0.1322 | -0.3418 | -0.4884 |  |  |
| 4-Methoxybenzyl alcohol |  | 1.9402 | 1.4758 | 1.1475 | 0.8375 | -0.1268 | -0.3571 | -0.5726 | -0.7346 | -0.9030 | -1.1210 |  |  |
| 4-Methylphenol |  |  |  |  |  | -0.5793 | -0.7788 |  |  |  |  |  |  |
| 4-Nitroaniline |  |  |  |  |  | 0.5050 | 0.2181 | -0.0291 | -0.2529 | -0.4510 |  |  |  |
| 4-Nitrobenzyl alcohol |  |  |  | 1.7055 | 1.3462 | 0.3492 | 0.0701 | -0.1726 | -0.3848 | -0.5530 | -0.7152 | 0.8000 | -0.9810 |
| 4-Nitrotoluene |  |  |  |  |  | -0.2231 | -0.4331 | -0.6288 | -0.8104 | -0.9364 |  |  |  |
| 4-Phenylphenol |  |  |  |  |  | 0.6954 | 0.3843 | 0.1127 | -0.1274 | -0.3434 |  |  |  |
| 4,4'-Dibromobiphenyl |  |  |  |  |  |  |  | 0.6396 | 0.3700 | 0.1279 | -0.0931 | -0.2830 | -0.4520 |
| 8-Hydroxyquinoline |  |  |  |  |  |  |  | -0.3259 | -0.5390 | -0.6953 | -0.8628 | -0.9655 | -1.1020 |
| Acenaphthene |  |  |  |  |  |  |  |  |  |  | -0.7574 | -0.9130 | -0.9559 |
| Acenaphthylene |  |  |  |  |  | 0.3025 | 0.0432 | -0.1906 | -0.3954 | -0.5772 | -0.7686 | -0.9460 | -0.9810 |
| Acetamide | 0.8119 | 0.3901 | 0.1066 | -0.1773 |  |  |  |  |  |  |  |  |  |
| Acetophenone |  | 1.2670 | 0.9285 | 0.6337 | 0.3759 | -0.5377 | -0.7281 | -0.8971 |  |  |  |  |  |
| alpha-Isomethyl ionone |  |  | 1.9584 | 1.6024 | 1.2530 | 0.2636 | -0.0057 | -0.2495 | -0.4501 | -0.6403 | -0.8041 |  |  |
| alpha-Pinene | 1.2290 | 0.8630 | 0.5657 | 0.3076 | 0.0731 | -0.8122 | -1.0056 | -1.1498 | -1.3143 | -1.4057 |  |  |  |
| Amyl cinnamal |  |  | 2.3803 | 1.9896 | 1.5989 | 0.5767 | 0.2742 | 0.0043 | -0.2196 | -0.4303 | -0.6168 |  | -0.8800 |
| Androsterone |  |  |  |  |  |  |  | 1.2951 | 0.9635 | 0.6721 | 0.4178 | 0.1810 | 0.0436 |
| Aniline |  | 0.9950 | 0.6820 | 0.4086 | 0.1708 | -0.7199 | -0.8949 |  |  |  |  |  |  |
| Anisole |  |  |  |  |  | -0.8568 |  |  |  |  |  |  |  |
| Anthracene |  |  |  |  |  | 0.8419 | 0.5406 | 0.2734 | 0.0341 | -0.1780 | -0.3567 | -0.5315 | -0.6404 |
| Anthraquinone |  |  |  |  |  |  |  | 0.6075 | 0.3434 | 0.1098 | -0.0988 | -0.2814 | -0.4545 |
| Azulene |  |  |  |  |  |  |  | -0.3805 | -0.6058 | -0.7617 | -0.9420 | -1.0251 | -1.1613 |
| Benz[a]anthracene |  |  |  |  |  |  |  | 1.2379 | 0.9261 | 0.6494 | 0.4020 | 0.1750 | -0.0121 |
| Benzaldehyde | 1.2965 | 0.9440 | 0.6391 | 0.3730 | 0.1403 | -0.7476 | -0.9128 |  |  |  |  |  |  |
| Benzamide |  |  |  |  |  | -0.0236 | -0.2678 | -0.4698 | -0.6747 | -0.8184 |  |  |  |
| Benzene | 0.2581 | 0.0050 | -0.2101 | -0.4000 | -0.5680 |  |  |  |  |  |  |  |  |
| Benzenesulfonamide |  |  |  |  |  | 0.3934 | 0.1161 | -0.1328 | -0.3494 | -0.5313 | -0.6932 | -0.8000 | -0.9140 |
| Benzidine |  |  |  |  |  |  |  | 0.7912 | 0.5027 | 0.2452 | -0.0212 | -0.2393 | -0.3670 |
| Benzo[a]pyrene |  |  |  |  |  |  |  | 1.7350 | 1.3843 | 1.0739 | 0.7995 | 0.5517 | 0.3226 |
| Benzo[e]pyrene |  |  |  |  |  |  |  | 1.7086 | 1.3672 | 1.0584 | 0.7819 | 0.5308 | 0.3103 |
| Benzo[ghi]perylene |  |  |  |  |  |  |  |  | 1.8401 | 1.5025 | 1.1851 | 0.8942 | 0.6099 |
| Benzophenone |  |  |  |  |  | 0.5509 | 0.2635 | 0.0073 | -0.2214 | -0.4205 |  |  |  |
| Benzothiazole |  |  |  |  |  |  |  | -0.5107 | -0.7459 | -0.8819 | -1.0635 | -1.1540 | -1.2540 |
| Benzyl 2-ethylhexyl phthalate |  |  |  |  |  |  |  | 1.3423 | 0.9670 | 0.6361 | 0.3482 | 0.0934 | -0.0818 |
| Benzyl alcohol |  |  |  |  |  | -0.6240 | -0.8148 | -0.9712 |  |  |  |  |  |
| Benzyl cinnamate |  |  |  |  |  | 1.3874 | 1.0124 | 0.6808 | 0.4494 | 0.1260 | -0.1100 |  | -0.4550 |
| Benzyl salicylate |  |  |  | 2.4688 | 2.0412 | 0.9916 | 0.6579 | 0.3624 | 0.1021 | -0.1290 | -0.3480 |  | -0.6476 |
| Bis(trimethylsiloxy)methylsilane | 0.9021 | 0.5113 | 0.2565 | 0.0037 |  |  |  |  |  |  |  |  |  |
| Borneol | 2.0585 | 1.5721 | 1.1741 | 0.8803 | 0.6058 | -0.3218 | -0.5346 | -0.7136 | -0.8931 | -1.0201 | -1.1974 |  |  |
| Butan-1-ol | 0.2408 | -0.0390 | -0.2746 | -0.4750 | -0.6540 |  |  |  |  |  |  |  |  |
| Butyl acetate | 0.7818 | 0.4540 | 0.1725 | -0.0710 | -0.2810 |  |  |  |  |  |  |  |  |
| Butyl benzyl phthalate |  |  |  |  |  |  |  |  |  |  | 0.1630 | -0.0662 | -0.2168 |
| Butyl cyclohexyl phthalate |  |  |  |  |  | 1.6336 | 1.2315 | 0.8750 | 0.5617 | 0.2828 | 0.0254 | -0.1860 | -0.3187 |
| Butyl decyl phthalate |  |  |  |  |  | 1.1582 | 0.7924 | 0.4688 | 0.1898 | -0.0711 | -0.3079 | -0.4468 | -0.6130 |
| Butyl octyl phthalate |  |  |  |  |  | 1.1611 | 0.7954 | 0.5253 | 0.1851 | -0.0671 |  | -0.4931 |  |
| Butyl oleate |  |  |  |  |  | 1.9091 | 1.4602 | 1.0651 | 0.7146 | 0.4037 | 0.1270 | -0.1197 | -0.2738 |
| Butyl stearate |  |  |  |  |  |  |  |  | 0.7494 | 0.4311 | 0.1478 | -0.1038 | -0.2618 |
| Camphor | 1.9726 | 1.5056 | 1.1219 | 0.8347 | 0.5685 | -0.3587 | -0.5597 | -0.7477 | -0.9124 | -1.0305 | -1.1974 |  |  |
| Carbazole |  |  |  |  |  | 0.9222 | 0.6058 | 0.3276 | 0.0759 | -0.1433 | -0.3249 | -0.5020 | -0.6108 |
| Carbon tetrachloride | 0.2624 | 0.0070 | -0.2082 | -0.3970 | -0.5640 |  |  |  |  |  |  |  |  |
| Carvone | 2.3357 | 1.8044 | 1.3694 | 1.0548 | 0.7593 | -0.1881 | -0.4154 | -0.6210 | -0.8080 | -0.9446 | -1.1404 |  |  |
| Chlorobenzene | 0.9077 | 0.5970 | 0.3276 | 0.0911 | -0.1160 |  |  |  |  |  |  |  |  |
| Chloroform | 0.0855 | -0.1600 | -0.3664 | -0.5470 | -0.7080 |  |  |  |  |  |  |  |  |
| Cholestane |  |  |  |  |  |  |  | 1.6952 | 1.3190 | 0.9871 | 0.7048 | 0.4445 | 0.2794 |
| Cholesterol |  |  |  |  |  |  |  |  |  | 1.2657 | 0.9669 | 0.6794 | 0.4906 |
| Cholesteryl acetate |  |  |  |  |  |  |  |  | 1.8353 | 1.4189 | 1.1011 | 0.7946 | 0.5922 |
| Chrysene |  |  |  |  |  | 1.9122 | 1.5225 | 1.1757 | 0.8646 | 0.5875 | 0.3473 | 0.1262 | -0.0171 |
| Cinnamyl alcohol |  |  |  |  |  | -0.0763 | -0.3193 | -0.5241 | -0.7159 | -0.8651 |  |  |  |
| Citronellal | 2.0358 | 1.5333 | 1.1233 | 0.8129 | 0.5282 | -0.3974 | -0.6167 | -0.7977 | -0.9773 | -1.1194 |  |  |  |
| Coumarin |  |  |  |  |  | 0.2098 | -0.0426 | -0.2610 | -0.4605 | -0.6298 | -0.7919 | -0.9090 |  |
| Cyclohexanol | 1.0461 | 0.7050 | 0.4173 | 0.1690 | -0.0510 |  |  |  |  |  |  |  |  |
| Decamethylcyclopentasiloxane | 2.0439 | 1.5370 | 1.1429 | 0.7805 | 0.4677 |  |  |  |  |  |  |  |  |
| Decamethyltetrasiloxane | 1.7263 | 1.2523 | 0.8904 | 0.5541 | 0.2529 |  |  |  |  |  |  |  |  |
| Decan-1-ol |  |  |  |  |  | -0.1858 | -0.4287 | -0.6329 | -0.8337 | -0.9800 |  |  |  |
| Decane |  | 1.0530 | 0.7167 | 0.4232 | 0.1670 | -0.7370 | -0.9288 |  |  |  |  |  |  |
| Di-(2-Methoxyethyl) phthalate |  |  |  |  |  | 1.2370 | 0.8627 | 0.5318 | 0.2423 | -0.0234 | -0.2526 | -0.4468 | -0.5748 |
| Di-2-ethylhexyl phthalate |  |  |  |  |  |  | 1.7637 | 1.3455 | 0.9706 | 0.6401 | 0.3525 | 0.0926 | -0.0708 |
| Di-n-Butyl phthalate |  |  |  |  |  | 1.1671 | 0.7983 | 0.4741 | 0.1939 | -0.0599 | -0.2886 | -0.4931 | -0.6265 |
| Di-n-Butyl succinate |  |  |  |  |  | 0.3845 | 0.0823 | -0.1918 | -0.4156 | -0.6197 | -0.7949 |  | -1.0991 |
| Di-n-Octyl phthalate |  |  |  |  |  |  |  | 1.6192 | 1.2173 | 0.8619 | 0.5538 | 0.2781 | 0.1042 |
| Di(2-Ethoxyethyl) phthalate |  |  |  |  |  | 1.4616 | 1.0621 | 0.7083 | 0.3994 | 0.1219 | -0.1214 | -0.3337 | -0.4771 |
| Di(2-n-butoxyethyl) phthalate |  |  |  |  |  |  | 1.6469 | 1.2404 | 0.8772 | 0.5559 | 0.2754 | 0.0169 | -0.1411 |
| Dibenzofuran |  |  |  |  |  | 0.3565 | 0.0927 | -0.1422 | -0.3515 | -0.5379 |  |  |  |
| Dibenzyl ether |  |  | 2.3679 | 1.9865 | 1.6032 | 0.5848 | 0.2864 | 0.0218 | -0.2130 | -0.4333 | -0.6188 | -0.7821 | -0.9009 |
| Dibenzylamine |  |  |  |  |  | 0.7179 | 0.4064 | 0.1374 | -0.1069 | -0.3200 |  |  |  |
| Dicyclohexyl phthalate |  |  |  |  |  |  | 1.6704 | 1.2830 | 0.9372 | 0.6303 | 0.3544 | 0.1112 | -0.0314 |
| Dicyclohexylamine |  |  |  |  |  | 0.2210 | -0.0266 | -0.3274 | -0.4897 | -0.7022 | -0.8010 |  |  |
| Dicylcohexyl adipate |  |  |  |  |  | 1.7559 | 1.3406 | 0.9723 | 0.6469 | 0.3537 |  |  |  |
| Diethoxydimethylsilane | 0.6188 | 0.2649 | 0.0533 | -0.1625 |  |  |  |  |  |  |  |  |  |
| Diethyl adipate |  |  |  |  |  | 0.0303 | -0.2393 | -0.4828 | -0.6879 | -0.8705 |  | -1.2061 | -1.2925 |
| Diethyl diethylmalonate |  |  |  |  |  | -0.1699 | -0.4166 | -0.6043 | -0.8302 | -0.9790 | -1.1824 | -1.3030 |  |
| Diethyl phthalate |  |  | 2.2707 | 1.8816 | 1.4947 | 0.4750 | 0.1775 | -0.0844 | -0.3184 | -0.5418 | -0.7127 | -0.8426 | -0.9862 |
| Diethyl sebecate |  |  |  |  |  | 0.8343 | 0.4830 | 0.1734 | -0.0898 | -0.3271 | -0.5450 | -0.7369 | -0.8261 |
| Dihydrocholesterol |  |  |  |  |  |  |  |  | 1.6217 | 1.2741 | 0.9741 | 0.6854 | 0.5021 |
| Diisobutyl phalate |  |  |  |  |  | 0.9829 | 0.6370 | 0.3297 | 0.0547 | -0.1863 | -0.3712 | -0.5828 | -0.6931 |
| Dimethyl phthalate |  |  |  |  |  | 0.2114 | -0.0590 | -0.3022 | -0.4964 | -0.7036 | -0.8560 | -1.0170 | -1.1129 |
| Dioxane | 0.4085 | 0.1330 | -0.1029 | -0.3070 | -0.4850 |  |  |  |  |  |  |  |  |
| Diphenyl ether |  | 2.2597 | 1.7633 | 1.4264 | 1.0992 | 0.1266 | -0.1333 | -0.3494 | -0.5528 | -0.7257 | -0.9280 | -1.0656 | -1.1344 |
| Diphenylamine |  |  |  |  |  | 0.5310 | 0.2402 | -0.0162 | -0.2518 | -0.4463 | -0.5035 |  |  |
| Dodecamethylcyclohexasiloxane | 2.6745 | 2.1013 | 1.6458 | 1.2286 | 0.8816 |  |  |  |  |  |  |  |  |
| Dodecamethylpentasiloxane | 2.3953 | 1.8439 | 1.4087 | 1.0097 | 0.6745 |  |  |  |  |  |  |  |  |
| Dodecane |  |  |  | 0.9266 | 0.6207 |  |  | -0.7406 | -0.9207 |  |  |  |  |
| Dodecanol |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Ethyl acetate | 0.0551 | -0.2050 | -0.4256 | -0.6170 | -0.7890 |  |  |  |  |  |  |  |  |
| Ethyl oleate |  |  |  |  |  | 1.5541 | 1.1384 | 0.7724 | 0.4524 | 0.1678 | -0.1190 | -0.3140 | -0.4581 |
| Ethylbenzene | 0.9597 | 0.6370 | 0.3599 | 0.1174 | -0.0930 |  |  |  |  |  |  |  |  |
| Eugenol |  | 2.1524 | 1.6601 | 1.3196 | 0.9940 | 0.0197 | -0.2324 | -0.4574 | -0.6373 | -0.7796 | -1.0138 |  |  |
| Fluoranthene |  |  |  |  |  | 1.2892 | 0.9520 | 0.6492 | 0.3838 | 0.1377 | -0.0617 | -0.2501 | -0.3725 |
| Fluorene |  |  |  |  |  | 0.4785 | 0.2058 | -0.0371 | -0.2552 | -0.4456 | -0.6089 |  | -0.9053 |
| Geraniol |  | 1.8544 | 1.3929 | 1.0588 | 0.7490 | -0.2134 | -0.4529 | -0.6648 | -0.8570 | -0.9950 | -1.2051 |  |  |
| Glycidoxypropyltrimethoxysilane | 3.1077 | 2.5069 | 2.0231 | 1.5782 | 1.2090 |  |  |  |  |  | -0.9158 | -1.0600 |  |
| Heptanal | 1.0977 | 0.7470 | 0.4446 | 0.1818 | -0.0460 |  |  |  |  |  |  |  |  |
| Heptane | 0.3716 | 0.0920 | -0.1473 | -0.3560 | -0.5360 |  |  |  |  |  |  |  |  |
| Hexachlorobenzene |  |  |  |  |  | 0.7079 | 0.4155 | 0.1575 | -0.0761 | -0.2822 | -0.4661 | -0.6201 | -0.7206 |
| Hexadecane |  |  |  |  |  | 0.4573 | 0.1468 | -0.1283 | -0.3729 | -0.5882 |  |  |  |
| Hexaethylcyclotrisiloxane | 2.9085 | 2.3643 | 1.9030 | 1.4766 | 1.1241 |  |  |  |  |  |  |  |  |
| Hexamethylcyclotrisiloxane | 0.8182 | 0.4374 | 0.1987 | -0.0531 | -0.3343 |  |  |  |  |  |  |  |  |
| Hexamethyldisilane | 0.4861 | 0.1467 | -0.0153 | -0.2212 |  |  |  |  |  |  |  |  |  |
| Hexamethyldisilathiane | 1.2807 | 0.8971 | 0.6122 | 0.3377 | 0.0785 |  |  |  |  |  |  |  |  |
| Hexamethyldisilazane | 0.7214 | 0.3614 | 0.1480 | -0.0738 |  |  |  |  |  |  |  |  |  |
| Hexamethyldisiloxane | 0.3185 | -0.0427 | -0.2652 | -0.4571 |  |  |  |  |  |  |  |  |  |
| Hexanal | 0.7322 | 0.4180 | 0.1504 | -0.0840 | -0.2860 |  |  |  |  |  |  |  |  |
| Hexane | 0.0038 | -0.2420 | -0.4517 | -0.6370 | -0.8040 |  |  |  |  |  |  |  |  |
| Hexanol | 0.9835 | 0.6360 | 0.3342 | 0.0778 | -0.1490 |  |  |  |  |  |  |  |  |
| Hydroxycitronellal |  | 1.9529 | 1.4776 | 1.1396 | 0.8217 | -0.1451 | -0.3874 | -0.6006 | -0.7841 | -0.9403 |  |  |  |
| Iodobenzene |  |  |  |  |  | -0.5546 | -0.7402 |  |  |  |  |  |  |
| Isocyanatopropyltriethoxysilane |  | 2.1967 | 1.7436 | 1.3226 | 0.9700 |  |  |  |  |  | -1.0668 | -1.1983 |  |
| Lilial |  |  | 2.0793 | 1.7121 | 1.3496 | 0.3500 | 0.0693 | -0.1794 | -0.3964 | -0.5814 | -0.7801 |  |  |
| Limonene | 1.5721 | 1.1514 | 0.8096 | 0.5325 | 0.2843 | -0.6311 | -0.8261 | -0.9900 | -1.1697 | -1.2743 |  |  |  |
| Linalool | 1.8459 | 1.3695 | 0.9832 | 0.6833 | 0.4085 | -0.5250 | -0.7298 | -0.9018 | -1.1093 | -1.2559 |  |  |  |
| Methacryloxypropyltrimethoxysilane | 3.0312 | 2.4310 | 1.9503 | 1.5096 | 1.2080 | 0.1221 | -0.1626 | -0.4124 | -0.6234 | -0.8334 | -0.9621 | -1.1830 | -1.3030 |
| Methyl abietate |  |  |  |  |  |  | 1.3980 | 1.0361 | 0.7140 | 0.4258 | 0.1742 | -0.0560 | -0.1859 |
| Methyl decanoate |  |  |  |  | 0.9007 |  |  |  |  |  |  |  |  |
| Methyl eugenol |  |  | 1.7861 | 1.4246 | 1.0776 | 0.0874 | -0.1738 | -0.4142 | -0.6038 | -0.7965 | -1.0140 |  |  |
| Methyl hexanoate | 1.1787 | 0.8120 | 0.4876 | 0.2237 | -0.0350 |  |  |  |  |  |  |  |  |
| Methyl nonanoate |  | 1.7563 | 1.3052 | 0.9753 | 0.6899 | -0.2912 | -0.4749 | -0.6929 | -0.9084 | -1.0305 | -1.2290 |  |  |
| Methyl octanoate |  |  | 1.0610 | 0.7314 | 0.4420 |  |  |  |  |  |  |  |  |
| Methylbis(trimethylsiloxy)vinylsilane | 1.3035 | 0.8883 | 0.5789 | 0.2863 | 0.0052 |  |  |  |  |  |  |  |  |
| Methyltriethoxysilane | 1.0550 | 0.6549 | 0.3730 | 0.1129 | -0.1844 |  |  |  |  |  |  |  |  |
| Methyltris(trimethylsiloxy)silane | 1.6541 | 1.1903 | 0.8379 | 0.5091 | 0.2211 |  |  |  |  |  |  |  |  |
| N-Methylacetamide |  | 0.5364 | 0.2837 | 0.0630 | -0.2504 |  |  |  |  |  |  |  |  |
| N,N-Diethylcarbanilide |  |  |  | 2.5107 | 2.0794 |  | 0.6928 | 0.3946 | 0.1366 | -0.0899 | -0.3130 | -0.5010 | -0.5935 |
| N,N-Diethyldodecamide |  |  |  |  |  | 1.1323 | 0.7645 | 0.4392 | 0.1546 | -0.0963 | -0.3269 | -0.5520 | -0.6311 |
| N,N-Dimethyl-4-nitroaniline |  |  |  |  |  |  | 0.5121 | 0.1789 | 0.0295 | -0.2039 | -0.3646 |  |  |
| N,N-Dimethylaniline |  |  |  |  | 0.4701 |  |  |  |  |  |  |  |  |
| N,N-Diphenyl-4-phenylenediamine |  |  |  |  |  |  |  |  |  | 0.7938 | 1.4709 | 0.2731 | 0.1088 |
| Naphthalene |  |  |  |  |  | -0.2622 | -0.4720 | -0.6540 | -0.8381 | -0.9769 |  |  |  |
| Neral |  | 1.8930 | 1.4323 | 1.1019 | 0.7912 | -0.1692 | -0.4131 | -0.6191 | -0.8300 | -0.9713 |  |  |  |
| Nicotinamide |  |  | 1.7709 | 1.4143 | 1.0757 | 0.0923 | -0.1633 | -0.3892 | -0.5797 | -0.7449 | -0.8599 |  | -1.0923 |
| Nicotine |  | 2.0921 | 1.7036 | 1.2960 | 0.9842 | 0.0230 | -0.2168 | -0.4359 | -0.6134 | -0.7782 | -0.9158 | -1.0952 | -1.1649 |
| Nitrobenzene |  | 1.3330 | 0.9945 | 0.7303 | 0.4401 |  |  |  |  |  |  |  |  |
| Nonanal |  |  |  | 0.6976 | 0.4207 |  |  |  |  |  |  |  |  |
| Nonane | 1.0882 | 0.7360 | 0.4342 | 0.1664 | -0.0680 | -0.9429 |  |  |  |  |  |  |  |
| Octadecane |  |  |  |  |  | 0.8511 | 0.5026 | 0.1962 | -0.0772 | -0.3193 |  |  |  |
| Octaethylcyclotetrasiloxane |  |  |  | 2.2371 | 1.8100 |  |  |  |  |  |  |  |  |
| Octamethylcyclotetrasiloxane | 1.4639 | 1.0162 | 0.6843 | 0.3736 | 0.0802 |  |  |  |  |  |  |  |  |
| Octamethyltrisiloxane | 1.0364 | 0.6356 | 0.3619 | 0.0973 | -0.1973 |  |  |  |  |  |  |  |  |
| Octan-1-ol |  | 1.2790 | 0.9166 | 0.6029 | 0.3308 |  |  |  |  |  |  |  |  |
| Octanal | 1.4557 | 1.0670 | 0.7342 | 0.4436 | 0.1908 |  |  |  |  |  |  |  |  |
| Octane | 0.7338 | 0.4170 | 0.1461 | -0.0910 | -0.2970 |  |  |  |  |  |  |  |  |
| Octanophenone |  |  |  |  |  | 0.6153 | 0.3058 | 0.0310 | -0.2188 | -0.4290 | -0.5897 | -0.8003 | -0.8522 |
| Octyltriethoxysilane |  |  |  |  |  | 0.2097 | -0.0917 |  |  |  | -0.9710 | -1.0952 | -1.0360 |
| Pentachlorophenol |  |  |  |  |  | 0.7805 | 0.4759 | 0.2067 | -0.0301 | -0.2441 |  |  |  |
| Pentan-1-ol | 0.6162 | 0.3030 | 0.0376 | -0.1940 | -0.3930 |  |  |  |  |  |  |  |  |
| Pentan-2-ol | 0.3623 | 0.0810 | -0.1526 | -0.3750 | -0.5550 |  |  |  |  |  |  |  |  |
| Pentan-3-ol | 0.3727 | 0.0890 | -0.1524 | -0.3640 | -0.5470 |  |  |  |  |  |  |  |  |
| Perylene |  |  |  |  |  |  |  |  | 1.3276 | 1.0159 | 0.7517 | 0.4993 | 0.3464 |
| Phenanthrene |  |  |  |  |  | 0.8249 | 0.5256 | 0.2601 | 0.0203 | -0.1883 | -0.3689 | -0.5248 | -0.6428 |
| Phenol | 1.3828 | 0.9850 | 0.6483 | 0.3602 | 0.1136 | -0.7810 |  |  |  |  |  |  |  |
| Phenylacetate |  |  |  |  |  | -0.5697 |  |  |  |  |  |  |  |
| Phenylcyclohexane |  |  |  |  |  | -0.0189 | -0.2578 | -0.4651 | -0.6511 |  | -0.9533 | -1.1471 | -1.1893 |
| Phenylsilane | 0.7036 | 0.3670 | 0.1701 | -0.0399 | -0.3299 |  |  |  |  |  |  |  |  |
| Phenyltrimethoxysilane | 2.2242 | 1.7282 | 1.3408 | 0.9749 | 0.6749 |  |  |  |  |  |  |  |  |
| Phthalimide |  |  |  |  |  | 0.2286 | -0.0343 | -0.2663 | -0.4708 | -0.6480 |  |  |  |
| Phthalonitrile |  |  |  |  |  | -0.0226 | -0.2678 | -0.4670 | -0.6702 | -0.8080 |  |  |  |
| Progesterone |  |  |  |  |  |  |  | 1.6807 | 1.3090 | 0.9889 | 0.7100 | 0.4567 | 0.2937 |
| Propyl acetate | 0.4194 | 0.1260 | -0.1230 | -0.3410 | -0.5280 |  |  |  |  |  |  |  |  |
| Pyrene |  |  |  |  |  | 1.3685 | 1.0278 | 0.7225 | 0.4546 | 0.2119 |  |  |  |
| Pyridine | 0.5364 | 0.2560 | 0.0152 | -0.1960 | -0.3790 |  |  |  |  |  |  |  |  |
| Quinoline |  |  |  |  |  | -0.1671 | -0.3886 | -0.5860 | -0.7652 |  | -1.0668 | -1.1983 | -1.3140 |
| Styrene | 1.0640 | 0.7330 | 0.4425 | 0.1930 | -0.0250 |  |  |  |  |  |  |  |  |
| p-Terphenyl |  |  |  |  |  |  |  | 0.8884 | 0.5942 | 0.3287 | 0.0927 | -0.1206 | -0.3091 |
| Terpinen-4-ol | 2.1049 | 1.6093 | 1.2053 | 0.9067 | 0.6182 | -0.3155 | -0.5331 | -0.7169 | -0.8931 | -1.0359 | -1.2209 |  |  |
| Tetraethylorthosilicate | 1.4319 | 0.9937 | 0.6679 | 0.3628 | 0.0715 |  |  |  |  |  |  |  |  |
| Tetrahydofuran | 0.1237 | -0.1230 | -0.3318 | -0.5160 | -0.6800 |  |  |  |  |  |  |  |  |
| Tetrakis(trimethylsiloxy)silane | 2.1605 | 1.6417 | 1.2362 | 0.8601 | 0.5527 |  |  |  |  |  |  |  |  |
| Tetramethylorthosilicate | 0.6723 | 0.3049 | 0.0921 | -0.1316 | -0.4759 |  |  |  |  |  |  |  |  |
| Thioacetamide |  |  |  | 0.4978 | 0.2778 |  |  |  |  |  | -0.5656 | -0.7961 |  |
| Toluene | 0.6326 | 0.3420 | 0.0928 | -0.1260 | -0.3150 |  |  |  |  |  |  |  |  |
| Trans Stilbene |  |  |  |  |  | 0.6960 | 0.3941 | 0.1249 | -0.1151 | -0.3261 | -0.5155 | -0.6700 | -0.7814 |
| Tri-n-Butyrin |  |  |  |  |  | 0.9556 | 0.5906 | 0.2721 | -0.0130 | -0.2613 | -0.4704 | -0.6542 | -0.7847 |
| Tribenzylamine |  |  |  |  |  | 1.7322 | 1.3287 | 0.9825 | 0.6559 | 0.3812 | 0.1266 | -0.0964 | -0.2350 |
| Tridecane |  |  |  |  | 0.8443 |  |  |  |  |  |  |  |  |
| Triethylamine | 0.3198 | 0.0470 | -0.1857 | -0.3920 | -0.5680 |  |  |  |  |  |  |  |  |
| Triisopropanolamine |  |  | 1.8974 | 1.5276 | 1.1644 | 0.1634 | -0.1134 | -0.3500 | -0.5637 | -0.7163 | -0.8851 |  |  |
| Tris(trimethylsiloxy)silane | 1.5531 | 1.0972 | 0.7542 | 0.4340 | 0.1382 |  |  |  |  |  |  |  |  |
| Trimethoprin |  |  |  |  |  |  |  |  |  |  | 0.4667 | 0.2170 | 0.0524 |
| Triphenylamine |  |  |  |  |  | 1.2706 | 0.9133 | 0.5987 | 0.3164 | 0.0656 | -0.1512 | -0.3422 | -0.4519 |
| Triphenylene |  |  |  |  |  |  |  |  |  |  | 0.4240 | 0.1965 | -0.0144 |
| Triphenylmethane |  |  |  |  |  | 1.2313 | 0.8764 | 0.5633 | 0.2832 | 0.0342 | -0.1802 | -0.3783 | -0.4787 |
| Undecane |  |  | 0.9975 | 0.6722 | 0.3970 | -0.5388 | -0.7437 | -0.9204 |  |  |  |  |  |
| Valeraldehyde | 0.3612 | 0.0840 | -0.1524 | -0.3590 | -0.5400 |  |  |  |  |  |  |  |  |
| Valerophenone |  |  |  |  |  | 0.0212 | -0.2922 | -0.4550 | -0.6540 | -0.8291 | -0.9895 | -1.1014 | -1.1893 |
| Vanillin |  | 2.2702 | 1.7631 | 1.4177 | 1.0876 | 0.1107 | -0.1401 | -0.3644 | -0.5655 | -0.7265 | -0.9239 |  |  |

Table S-3

Retention factor database for Rxi-17 (60-260 °C)

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| compound | log60 | log80 | log100 | log120 | log140 | log160 | log180 | log200 | log220 | log240 | log260 |
| 1-Acetonaphthone |  |  |  |  |  | 1.2166 | 0.9066 | 0.6321 | 0.3837 | 0.1592 | -0.0378 |
| 1-Bromododecane |  |  |  |  |  | 0.6910 | 0.3988 | 0.1338 | -0.1051 | -0.3173 |  |
| 1-Bromonaphthalene |  |  |  |  |  | 0.9703 | 0.6975 | 0.4498 | 0.2275 | 0.0194 |  |
| 1-Chloronaphthalene |  |  |  |  |  | 0.7369 | 0.4786 | 0.2438 | 0.0271 | -0.1710 |  |
| 1-Hexyne | -0.3519 | -0.7224 |  |  |  |  |  |  |  |  |  |
| 1-Naphthol |  |  |  |  |  | 1.0584 | 0.7668 | 0.5039 | 0.2691 | 0.0534 | -0.1185 |
| 1-Nitronaphthalene |  |  |  |  |  | 1.2600 | 0.9537 | 0.6808 | 0.4361 | 0.2128 | 0.0226 |
| 1-Nitropropane | 0.5373 | 0.1931 | -0.1117 | -0.4011 | -0.6654 |  |  |  |  |  |  |
| 1-Phenylethanol |  | 1.3165 | 0.9338 | 0.5971 | 0.3014 |  |  |  |  |  |  |
| 1-Phenyl-1-propanol |  |  | 1.1593 | 0.8071 | 0.4927 |  |  |  |  |  |  |
| 1-Phenyl-2-propanol |  | 1.5153 | 1.0964 | 0.7467 | 0.4382 |  |  |  |  |  |  |
| 1,12-dodecanediol |  |  |  |  |  | 1.3115 | 0.9484 | 0.6359 | 0.3580 | 0.1082 |  |
| 1,2-Dichlorobenzene | 1.4664 | 1.0760 | 0.7387 | 0.4399 | 0.1726 | -0.1072 | -0.3167 | -0.5055 | -0.6783 | -0.8503 |  |
| 1,2-Dimethylbenzene | 0.8781 | 0.5264 | 0.2195 | -0.0531 | -0.3022 |  |  |  |  |  |  |
| 1,2,4,5-Tetrachlorobenzene |  |  | 1.4786 | 1.1188 | 0.7995 |  |  |  |  |  |  |
| 1,2,4-Trichlorobenzene |  | 1.4770 | 1.1133 | 0.7826 | 0.4899 |  |  |  |  |  |  |
| 1,3-Dibromobenzene |  |  | 1.2087 | 0.8734 | 0.5831 |  |  |  |  |  |  |
| 1,3-Dichlorobenzene | 1.3057 | 0.9261 | 0.5988 | 0.3074 | 0.0487 |  |  |  |  |  |  |
| 1,3-Dihydroxybenzene |  |  |  | 1.2098 | 0.8629 | 0.5523 | 0.2839 | 0.0141 | -0.1854 | -0.3658 |  |
| 1,3-Dimethylbenzene | 0.7670 | 0.4176 | 0.1168 | -0.1556 | -0.4025 | -0.5781 | -0.7869 | -1.0104 |  |  |  |
| 1,3-Dinitrobenzene |  |  |  |  |  | 0.9674 | 0.6739 | 0.4099 | 0.1716 | -0.0440 |  |
| 1,3,5-Triethylbenzene |  |  |  |  |  | 0.1021 | -0.1485 | -0.3751 | -0.5747 | -0.7604 |  |
| 1,4-Dimethylbenzene | 0.7583 | 0.4092 | 0.1085 | -0.1632 | -0.4098 |  |  |  |  |  |  |
| 2-(1-naphthyl)ethanol |  |  |  |  |  | 1.3856 | 1.0741 | 0.7874 | 0.5301 | 0.2961 |  |
| 2-Acetonaphthone |  |  |  |  |  | 1.2397 | 0.9309 | 0.6544 | 0.4068 | 0.1801 | -0.0358 |
| 2-Chloroaniline |  | 1.5279 | 1.1579 | 0.8209 | 0.5231 |  |  |  |  |  |  |
| 2-Chlorophenol | 1.3637 | 0.9776 | 0.6459 | 0.3512 | 0.0851 |  |  |  |  |  |  |
| 2-Ethoxyethanol | 0.3061 | -0.0350 | -0.3308 | -0.6054 | -0.8502 |  |  |  |  |  |  |
| 2-Heptanone | 0.8513 | 0.4745 | 0.1475 | -0.1417 | -0.4081 |  |  |  |  |  |  |
| 2-Hexanone | 0.5041 | 0.1280 | -0.1579 | -0.4519 | -0.6467 |  |  |  |  |  |  |
| 2-Methoxyethanol | 0.0591 | -0.2788 | -0.5845 | -0.8959 |  |  |  |  |  |  |  |
| 2-Methoxynaphthalene |  |  |  |  |  | 0.8708 | 0.5925 | 0.3371 | 0.1102 | -0.0928 |  |
| 2-Methylbutan-1-ol | 0.2809 | -0.0701 | -0.3872 | -0.6851 | -0.9778 |  |  |  |  |  |  |
| 2-Methyl-2-butanol | -0.1433 | -0.5085 |  |  |  |  |  |  |  |  |  |
| 2-Methylaniline |  |  |  |  |  | 0.0206 | -0.1526 | -0.3630 | -0.5520 | -0.7151 |  |
| 2-Methylnaphthalene |  |  |  |  |  | 0.4873 | 0.2386 | 0.0149 | -0.1836 | -0.3639 |  |
| 2-Methylphenol |  | 1.2202 | 0.8479 | 0.5230 | 0.2854 | -0.0675 | -0.2988 | -0.5009 | -0.6770 | -0.8522 |  |
| 2-Naphthol |  |  |  |  |  | 1.0633 | 0.7693 | 0.5060 | 0.2688 | 0.0563 | -0.1111 |
| 2-Nitroaniline |  |  |  |  |  | 0.9142 | 0.6320 | 0.3806 | 0.1519 | -0.0552 |  |
| 2-Nitrophenol |  | 1.4379 | 1.0640 | 0.7348 | 0.4440 | 0.1631 | -0.0661 | -0.2691 | -0.4527 | -0.6201 |  |
| 2-Nitropropane | 0.3570 | 0.0223 | -0.2751 | -0.5554 | -0.7971 |  |  |  |  |  |  |
| 2-Nonanone | 1.5342 | 1.0799 | 0.7513 | 0.4113 | 0.1103 |  |  |  |  |  |  |
| 2-Octanone | 1.1932 | 0.7854 | 0.4336 | 0.1203 | -0.1565 |  |  |  |  |  |  |
| 2-Pentanone | 0.1017 | -0.2108 | -0.5205 | -0.8032 |  |  |  |  |  |  |  |
| 2-Phenylethanol |  |  |  |  |  | 0.1313 | -0.1078 | -0.3267 | -0.5219 | -0.6968 |  |
| 2-Phenyl-1-propanol |  |  | 1.2538 | 0.8907 | 0.5678 |  |  |  |  |  |  |
| 2-Undecanone |  |  | 1.2821 | 0.9085 | 0.5666 | 0.2099 | -0.0560 | -0.3041 | -0.5267 | -0.7297 |  |
| 2,3-Dimethylphenol |  |  | 1.1534 | 0.8056 | 0.4988 |  |  |  |  |  |  |
| 2,6-Dimethylphenol |  | 1.3177 | 0.9442 | 0.6155 | 0.3275 |  |  |  |  |  |  |
| 3-Aminopropyltriethoxysilane | |  |  |  |  | 0.1207 | -0.1444 | -0.3925 | -0.6054 | -0.8200 |  |
| 3-Methylaniline |  |  |  |  |  | 0.0821 | -0.1539 | -0.3663 | -0.5520 | -0.7223 |  |
| 3-Methylbutanol | 0.2813 | -0.0754 | -0.3947 | -0.6931 | -0.9659 |  |  |  |  |  |  |
| 3-Methylphenol |  | 1.2845 | 0.9031 | 0.5698 | 0.2782 | -0.0174 | -0.2586 | -0.4650 | -0.6435 | -0.8187 |  |
| 3-Nitroaniline |  |  |  |  |  | 1.0974 | 0.8008 | 0.5354 | 0.2975 | 0.0783 | -0.1067 |
| 3-Nitrophenol |  |  |  |  | 1.2879 |  |  |  |  |  |  |
| 3-Phenylpropan-1-ol |  |  | 1.4170 | 1.0334 | 0.7050 |  |  |  |  |  |  |
| 3,4-Dichloroanilne |  |  |  |  |  | 0.9042 | 0.6242 | 0.3725 | 0.1459 | -0.0570 |  |
| 3,5-Dimethylphenol |  | 1.4609 | 1.0741 | 0.7225 | 0.4276 | 0.1455 | -0.0970 | -0.3047 | -0.4912 | -0.6676 |  |
| 4-acetylbiphenyl |  |  |  |  |  |  |  |  | 0.6983 | 0.4465 |  |
| 4-Chloroaniline |  |  |  |  |  | 0.3992 | 0.1509 | -0.0698 | -0.2664 | -0.4428 |  |
| 4-Chlorophenol |  |  | 1.2385 | 0.8864 | 0.5721 | 0.2795 | 0.0319 | -0.1879 | -0.3807 | -0.5540 |  |
| 4-Fluoroaniline | 1.5448 | 1.1370 | 0.7784 | 0.4616 | -0.0260 |  |  |  |  |  |  |
| 4-Hydroxybenzaldehyde |  |  |  |  | 1.0598 | 0.7361 | 0.4599 | 0.2102 | -0.0164 | -0.2177 |  |
| 4-Hydroxybezyl alcohol |  |  |  |  |  | 0.7171 | 0.4387 | 0.1899 | -0.0355 | -0.2344 |  |
| 4-Methylphenol | 1.2917 | 0.9138 | 0.5771 | 0.2823 | -0.0102 | -0.2559 | -0.4804 | -0.6447 | -0.8187 |  |  |
| 4-Nitroaniline |  |  |  |  |  | 1.4178 | 1.1077 | 0.8128 | 0.5546 | 0.3216 | 0.1024 |
| 4-Nitrotoluene |  |  |  |  |  | 0.3585 | 0.1102 | -0.1094 | -0.3005 | -0.4804 |  |
| 4-Phenylphenol |  |  |  |  |  |  |  |  | 0.5598 | 0.3190 | 0.1084 |
| Acenaphthylene |  |  |  |  |  | 0.9498 | 0.6734 | 0.4229 | 0.1963 | -0.0037 |  |
| Acetophenone | #NULL! | 1.3342 | 0.9593 | 0.6325 | 0.3389 | 0.0373 | -0.2012 | -0.4114 | -0.5931 | -0.7668 | -0.8437 |
| Aniline | 1.5068 | 1.0942 | 0.7442 | 0.4335 | 0.1564 | -0.1310 | -0.3556 | -0.5490 | -0.7251 | -0.8978 |  |
| Anisole |  |  |  |  |  | -0.4291 | -0.6414 | -0.8600 |  |  |  |
| Anthracene |  |  |  |  |  |  |  |  | 0.6929 | 0.4585 | 0.2451 |
| Benzaldehyde | 1.3630 | 0.9729 | 0.6342 | 0.3335 | 0.0663 | -0.2287 | -0.4384 | -0.6306 |  |  |  |
| Benzamide |  |  |  |  | 1.1587 | 0.7881 | 0.5189 | 0.2667 | 0.0399 | -0.1673 | -0.3342 |
| Benzene | 0.0329 | -0.2855 | -0.5507 | -0.7908 | -1.0466 |  |  |  |  |  |  |
| Benzenesulfonamide |  |  |  |  |  | 1.3666 |  | 0.7501 | 0.4935 | 0.2613 |  |
| Benzodioxane |  |  | 1.2650 | 0.9345 | 0.6260 |  |  |  |  |  |  |
| Benzonitrile | 1.5458 | 1.1446 | 0.7896 | 0.4773 | 0.1965 |  |  |  |  |  |  |
| Benzophenone |  |  |  |  |  | 1.2763 | 0.9593 | 0.6760 | 0.4223 | 0.1915 | -0.0020 |
| Benzyl alcohol |  | 1.2467 | 0.8747 | 0.5481 | 0.2575 | -0.0475 | -0.2782 | -0.4804 | -0.6548 | -0.8182 |  |
| Borneol |  | 1.3713 | 0.9965 | 0.6661 | 0.3785 |  |  |  |  |  |  |
| Bromobenzene | 1.1251 | 0.7664 | 0.4513 | 0.1600 | -0.0960 |  |  |  |  |  |  |
| Butan-1-ol | 0.0530 | -0.3062 | -0.6503 | -1.0605 |  |  |  |  |  |  |  |
| n-Butylbenzene | 1.3815 | 0.9805 | 0.6311 | 0.3082 | 0.0465 |  |  |  |  |  |  |
| Butyl acetate | 0.5390 | 0.1778 | -0.1426 | -0.4409 | -0.7138 |  |  |  |  |  |  |
| Butyl benzoate |  |  |  | 1.2725 | 0.9124 |  |  |  |  |  |  |
| Butyl benzyl phthalate |  |  |  |  |  |  |  |  |  |  | 0.8312 |
| Butyl cyclohexyl phalate |  |  |  |  |  |  |  |  |  |  | 0.2327 |
| Butyl decyl phthalate |  |  |  |  |  |  |  |  |  |  | 0.2362 |
| Butyl 2-ethylhexyl phthalate |  |  |  |  |  |  |  |  |  |  | 0.8144 |
| Camphor |  | 1.3830 | 1.0073 | 0.6766 | 0.3929 |  |  |  |  |  |  |
| Carbazole |  |  |  |  |  |  |  |  | 0.8320 | 0.5820 |  |
| Carbon tetrachloride | -0.0776 | -0.3799 | -0.6326 |  |  |  |  |  |  |  |  |
| Carvone |  |  | 1.3483 | 0.9840 | 0.6596 |  |  |  |  |  |  |
| Chlorobenzene | 0.7614 | 0.4236 | 0.1291 | -0.1358 | -0.3752 |  |  |  |  |  |  |
| Chloroform | -0.1754 | -0.4985 | -0.7758 |  |  |  |  |  |  |  |  |
| Cholesterol |  |  |  |  |  |  |  |  |  |  | 1.4387 |
| Chrysene |  |  |  |  |  |  |  |  |  |  | 1.0769 |
| Cinnamyl alcohol |  |  |  | 1.2305 | 0.8842 | 0.5717 | 0.3049 | 0.0623 | -0.1594 | -0.3556 |  |
| Coumarin | 0.9652 | 0.5850 | 0.2608 | -0.0497 | -0.2866 | 0.9935 | 0.7081 | 0.4518 | 0.2217 | 0.0097 |  |
| Cyclohexanone oxime |  |  |  |  |  | -0.0724 | -0.2988 | -0.4857 |  |  |  |
| Decamethylcyclopentasiloxane | |  | 1.1975 | 0.8160 | 0.4815 |  |  |  |  |  |  |
| Decamethyltetrasiloxane | 0.8532 | 0.4759 | 0.1412 | -0.1542 | -0.4325 |  |  |  |  |  |  |
| Decan-1-ol |  |  |  |  |  | 0.1360 | -0.1235 | -0.3545 | -0.5561 | -0.7478 |  |
| Di-2-ethylhexyl phthalate |  |  |  |  |  |  |  |  |  |  | 0.8150 |
| Dibenzofuran |  |  |  |  |  | 0.9846 | 0.7038 | 0.4521 | 0.2197 | 0.0159 |  |
| Dibenzyl ether |  |  |  |  |  | 1.1826 | 0.9356 | 0.6537 | 0.3956 | 0.1613 |  |
| Dibenzylamine |  |  |  |  |  | 1.3917 | 1.0217 | 0.7984 | 0.5175 | 0.2663 |  |
| Dicyclohexylamine |  |  |  |  |  | 0.5446 | 0.2828 | 0.0466 | -0.1697 | -0.3626 |  |
| Diethyl phthalate |  |  |  |  |  |  |  |  |  |  | -0.1583 |
| Dihydrocholesterol |  |  |  |  |  |  |  |  |  |  | 1.4332 |
| Diisobutyl phthalate | 0.3175 | -0.0129 | -0.3144 | -0.5735 | -0.8134 |  |  |  | 0.6313 | 0.3626 |  |
| Dimethyl phthalate |  |  |  |  |  |  |  |  |  |  | -0.2908 |
| Dodecamethylcyclohexasiloxane | 1.5005 | 1.0857 | 0.7124 | 0.3731 | 0.0677 |  |  |  |  |  |  |
| Dodecane | -0.2232 | -0.5927 |  |  |  | -0.2437 | -0.4825 | -0.6968 | -0.9088 |  | -1.1307 |
| Dodecanol |  |  | 1.1617 | 0.8101 | 0.4978 |  |  |  |  |  |  |
| Ethyl acetate | 0.6317 | 0.2642 | -0.0641 | -0.3593 | -0.6062 |  |  |  |  |  |  |
| Ethyl 2-methylbutyrate | 0.1589 | -0.1903 | -0.4965 | -0.7652 |  |  |  |  |  |  |  |
| Ethyl oleate | 0.7531 | 0.4063 | 0.1053 | -0.1651 | -0.4106 |  |  |  |  |  |  |
| Fluorene |  |  |  |  |  | 1.1352 | 0.8417 | 0.5808 | 0.3455 | 0.1297 |  |
| Geraniol |  |  | 0.9259 | 0.5200 | 0.1668 |  |  |  |  |  |  |
| Glycidoxypropyltrimethoxysilane | -0.2639 | -0.6166 | -0.9529 |  |  | 0.6483 | 0.4179 | 0.1372 | -0.1134 | -0.3360 |  |
| Hexachlorobenzene |  |  |  |  |  | 1.2683 | 0.9664 | 0.6963 | 0.4532 | 0.2289 |  |
| Hexadecane |  |  |  |  |  | 0.5714 | 0.2740 | 0.0059 | -0.2391 | -0.4600 | -0.6383 |
| Hexamethyldisilazane |  | 1.1080 | 0.6237 | 0.2824 |  |  |  |  |  |  |  |
| Hexanal | 0.7990 | 0.4042 | 0.0782 | -0.2236 | -0.5138 |  |  |  |  |  |  |
| Hexanol | 1.5235 | 1.1331 | 0.7963 | 0.4992 | 0.2347 |  |  |  |  |  |  |
| Iodobenzene |  |  |  |  |  | -0.0307 | -0.2434 | -0.4335 | -0.6021 | -0.7620 |  |
| Isocyanatopropyltriethoxysilane | |  |  |  |  | 0.2931 | 0.0028 | -0.2580 | -0.4842 | -0.6860 |  |
| Lilial |  | 1.1188 | 0.7317 | 0.4010 | 0.1055 |  |  |  |  |  |  |
| Methacryloxypropyltrimethoxysilane | | 1.3713 | 0.9889 | 0.6575 | 0.3608 | 0.5763 | 0.2716 | 0.0362 | -0.2470 | -0.4656 |  |
| Methyl abietate | 0.0064 | -0.3055 | -0.5819 | -0.8334 | -1.2080 |  |  |  |  |  |  |
| Methyl benzoate |  |  | 1.3073 | 0.9154 | 0.5686 |  |  |  |  |  |  |
| Methyl decanoate | 0.9269 | 0.5386 | 0.2025 | -0.0980 | -0.3736 |  |  |  |  |  |  |
| Methyl eugenol |  | 1.4889 | 1.0704 | 0.7018 | 0.3731 |  |  |  |  |  |  |
| Methyl hexanoate |  | 1.1575 | 0.7691 | 0.4262 | 0.1208 |  |  |  |  |  |  |
| N,N-Dimethylaniline |  |  | 1.1996 | 0.8672 | 0.5678 |  |  |  |  |  |  |
| Naphthalene |  |  |  |  |  | 0.2931 | 0.0553 | -0.1485 | -0.3332 | -0.5027 |  |
| Nicotinamide |  | 1.4069 | 1.0365 | 0.7113 | 0.4219 |  |  |  |  |  |  |
| Nicotine |  |  | 1.4507 | 1.0211 | 0.6319 |  |  |  |  |  |  |
| Nitrobenzene | 0.5260 | 0.1715 | -0.1478 | -0.4328 | -0.7121 |  |  |  |  |  |  |
| Octadecane |  |  |  |  |  | 0.9502 | 0.6183 | 0.3202 | 0.0548 | -0.1899 | -0.4005 |
| Octamethylcyclotetrasiloxane | 1.4589 | 1.0176 | 0.6405 | 0.3050 | 0.0116 |  |  |  |  |  |  |
| Octamethyltrisiloxane | 1.1978 | 0.7776 | 0.4216 | 0.1036 | -0.1766 |  |  |  |  |  |  |
| Octan-1-ol |  |  | 1.1640 | 0.7348 | 0.3699 |  |  |  |  |  |  |
| Octan-2-ol | 0.1408 | -0.1985 | -0.5667 | -0.7929 |  |  |  |  |  |  |  |
| Octanophenone |  |  |  |  |  | 1.1377 | 0.8116 | 0.5219 | 0.2618 | 0.0233 |  |
| Octyltriethoxysilane | 0.4324 | 0.0622 | -0.2588 | -0.5554 | -0.8390 |  |  |  |  |  |  |
| Pentachlorophenol | 0.1026 | -0.2487 | -0.5806 | -0.8959 |  |  |  |  | 0.5559 | 0.3251 | 0.1354 |
| Pentan-1-ol | 0.1159 | -0.2323 | -0.5654 | -0.8959 |  |  |  |  |  |  |  |
| Perylene | 1.2700 | 0.9368 | 0.5845 | 0.2807 | 0.0097 |  |  |  |  |  | 1.5651 |
| Phenanthrene |  | 1.2593 | 0.8802 | 0.5488 | 0.2526 |  |  |  | 0.6817 | 0.4486 | 0.2449 |
| Phenol |  |  |  |  |  | -0.2544 | -0.4702 | -0.6691 |  |  |  |
| Phenylacetate |  |  |  |  |  | -0.0598 | -0.2947 | -0.5064 | -0.6990 | -0.8807 |  |
| Phenylcyclohexane |  |  |  |  |  | 0.4321 | 0.1525 | -0.0455 | -0.2465 | -0.4292 |  |
| Phthalimide |  |  |  |  |  | 1.0327 | 0.7353 | 0.4703 | 0.2329 | 0.0167 |  |
| Phthalonitrile | 0.1733 | -0.1780 | -0.5008 | -0.7848 |  | 0.7612 | 0.4854 | 0.2378 | 0.0131 | -0.1899 |  |
| Propyl acetate | 0.5234 | 0.1920 | -0.1013 | -0.3777 | -0.6233 |  |  |  |  |  |  |
| Pyrene |  |  |  |  |  |  |  |  |  |  | 0.6941 |
| Quinine | 0.9257 | 0.5680 | 0.2571 | -0.0191 | -0.2732 |  |  |  |  |  |  |
| Quinoline |  |  |  |  |  | 0.4865 | 0.2398 | 0.0141 | -0.1854 | -0.3664 |  |
| Styrene |  | 1.3713 | 0.9920 | 0.6575 | 0.3621 |  |  |  |  |  |  |
| n-Tetradecane | -0.1111 | -0.4526 | -0.7372 | -1.0385 |  |  |  |  |  |  |  |
| Tetramethylorthosilicate | 0.4099 | 0.0883 | -0.1981 | -0.4510 | -0.6759 |  |  |  |  |  |  |
| Trans Stilbene |  |  |  |  |  |  |  | 0.7228 | 0.4637 | 0.2286 | 0.0216 |
| Tri-n-Butyrin |  | 1.3516 | 0.9760 | 0.0622 | 0.2971 |  |  | 0.7845 | 0.4518 | 0.1759 | -0.0761 |
| Tribenzylamine | -0.1683 | -0.5211 | -0.8318 |  |  |  |  |  |  |  |  |
| Triphenylamine |  |  |  |  |  |  |  |  |  | 0.7397 |  |
| Triphenylene | 1.1861 | 0.7924 | 0.4357 | 0.1249 | -0.1695 |  |  |  |  |  |  |
| Triphenylmethane | 1.2006 | 0.7077 | 0.2906 | -0.0682 | -0.3820 |  |  |  |  | 0.7039 | 0.4625 |
| Undecane |  |  |  |  |  |  | -0.7234 |  |  |  |  |
| Valerophenone |  |  |  |  |  | 0.5604 | 0.2887 | 0.0429 | -0.1819 | -0.3861 | -0.5266 |

Table S-4

Retention factor database for Rxi-5Sil MS (60-320 °C)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | log60 | log80 | log100 | log120 | log140 | log160 | log180 | log200 | log220 | log240 | log260 | log280 | log300 | log320 |
| 1-Acetonaphthone |  |  |  |  |  | 0.8796 | 0.5903 | 0.3354 | 0.1045 | -0.1077 | -0.2982 | -0.4439 | -0.6010 | -0.6348 |
| 1-Bromododecane |  |  |  |  |  | 0.7969 | 0.4981 | 0.2303 | -0.0127 | -0.2286 |  |  |  | -0.8820 |
| 1-Bromonaphthalene |  |  |  |  |  | 0.7203 | 0.4591 | 0.2205 | 0.0090 | -0.1951 |  |  |  |  |
| 1-Chloronaphthalene |  |  |  |  |  | 0.5227 | 0.2742 | 0.0481 | -0.1645 | -0.3541 |  |  |  |  |
| 1-Hydroxyanthraquinone | |  |  |  |  |  |  |  | 0.8140 | 0.5688 | 0.3128 | 0.1161 | -0.0799 | -0.2247 |
| 1-Methylnaphthalene |  |  | 1.3499 | 0.9963 | 0.6836 |  |  |  |  |  |  |  |  |  |
| 1-Naphthol |  |  |  |  | 1.0603 | 0.7291 | 0.4523 | 0.2037 | -0.0208 | -0.2229 | -0.3829 | -0.5126 |  |  |
| 1-Nitronaphthalene |  |  |  |  |  | 0.9051 | 0.6221 | 0.3683 | 0.1399 | -0.0662 | -0.2286 | -0.3887 |  |  |
| 1-Nitropropane | 0.2967 | -0.0392 | -0.3261 | -0.6141 | -0.9113 |  |  |  |  |  |  |  |  |  |
| 1-Nitropyrene |  |  |  |  |  |  |  |  | 1.4887 | 1.1956 | 0.8784 | 0.6398 | 0.4171 | 0.2193 |
| 1,12-dodecanediol |  |  |  |  |  | 1.1859 | 0.8443 | 0.5414 | 0.2728 | 0.0307 |  |  | -0.5370 | -0.7126 |
| 1,2-Dichlorobenzene | 1.2981 | 0.9173 | 0.5869 | 0.2923 | 0.0309 | -0.2512 | -0.4544 | -0.6372 | -0.8133 |  |  |  |  |  |
| 1,2-Dimethylbenzene | 0.8030 | 0.4594 | 0.1513 | -0.1195 | -0.3690 |  |  |  |  |  |  |  |  |  |
| 1,2,4,5-Tetrachlorobenzene | |  | 1.3485 | 0.9874 | 0.6741 |  |  | -0.1034 | -0.2914 | -0.4759 |  |  | -0.8523 | -0.9658 |
| 1,2,4-Trichlorobenzene | | 1.3560 | 0.9829 | 0.6569 | 0.3682 |  |  |  |  |  |  |  |  |  |
| 1,2,5,6-Dibenzoanthracene | |  |  |  |  |  |  |  | 2.3921 | 1.9217 | 1.6206 |  |  |  |
| 1,3-Dibromobenzene |  | 1.3871 | 1.0193 | 0.6898 | 0.4068 |  |  |  |  |  |  |  |  |  |
| 1,3-Dichlorobenzene | 1.1893 | 0.8186 | 0.4944 | 0.2047 | -0.0502 |  |  |  |  |  |  |  |  |  |
| 1,3-Dihydroxybenzene |  |  | 1.2445 | 0.8528 | 0.5219 | 0.2104 | -0.0192 | -0.2802 | -0.4760 | -0.6503 |  |  | -0.9870 | -0.9610 |
| 1,3-Dimethylbenzene | 0.7236 | 0.3806 | 0.0814 | -0.1913 | -0.4363 | -0.6383 | -0.8458 |  |  |  |  |  |  |  |
| 1,3-Dinitrobenzene |  |  |  |  |  | 0.5974 | 0.3310 | 0.0891 | -0.1276 | -0.3208 | -0.4716 | -0.6058 | -0.7411 | -0.8679 |
| 1,3,5-Triethylbenzene |  |  |  |  |  | 0.0846 | -0.1634 | -0.3857 | -0.5803 | -0.7628 |  |  |  |  |
| 1,4-Dimethylbenzene | 0.7278 | 0.3806 | 0.0822 | -0.1899 | -0.4355 |  |  |  |  |  |  |  |  |  |
| 2-(1-naphthyl)ethanol |  |  |  |  |  | 1.0312 | 0.7331 | 0.4670 | 0.2281 | 0.0087 | -0.1941 | -0.3545 | -0.5017 | -0.6216 |
| 2-Acetonaphthone |  |  |  |  |  | 0.9291 | 0.6406 | 0.3817 | 0.1497 | -0.0634 | -0.2497 | -0.4172 | -0.5773 | -0.6438 |
| 2-Chloroacetamide |  |  | 0.1372 |  | -0.3209 |  |  |  |  |  |  |  |  |  |
| 2-Chloroaniline |  | 1.2354 | 0.8685 | 0.5477 | 0.2636 |  |  |  |  |  |  |  |  |  |
| 2-Chlorophenol | 1.1855 | 0.8093 | 0.4783 | 0.2097 | -0.0747 |  |  |  |  |  |  |  | -1.2782 |  |
| 2-Ethoxyethanol | 0.1864 | -0.1505 | -0.4289 | -0.7052 |  |  |  |  |  |  |  |  |  |  |
| 2-Heptanone | 0.7974 | 0.4302 | 0.1123 | -0.1752 | -0.4289 |  |  |  |  |  |  |  |  |  |
| 2-Hexanone | 0.4255 | 0.1166 | -0.2131 | -0.5016 | -0.7640 |  |  |  |  |  |  |  |  |  |
| 2-Methoxycinnamaldehyde | |  |  |  |  | 0.7582 | 0.4683 | 0.2118 | -0.0226 | -0.2307 | -0.4101 | -0.5640 | -0.7113 | -0.8456 |
| 2-Methoxyethanol | -0.0926 | -0.4318 | -0.7496 |  |  |  |  |  |  |  |  |  |  |  |
| 2-Methoxynaphthalene | |  |  |  |  | 0.6195 | 0.3557 | 0.1116 | -0.1003 | -0.2920 |  |  |  | -0.8795 |
| 2-Methylbutan-1-ol | 0.2804 | -0.0744 | -0.3845 | -0.6866 | -0.9750 |  |  |  |  |  |  |  |  |  |
| 2-Methyl-2-butanol | -0.1101 | -0.4615 |  |  |  |  |  |  |  |  |  |  |  |  |
| 2-Methylaniline |  |  |  |  |  | -0.1671 | -0.3892 | -0.5835 | -0.7621 | -0.9171 |  |  |  |  |
| 2-Methylbenzothiazole |  |  |  |  |  |  |  | -0.1145 | -0.3351 | -0.4874 | -0.6209 | -0.7489 | -0.8695 | -0.9619 |
| 2-Methylnaphthalene |  |  |  |  |  | 0.3129 | 0.0719 | -0.1427 | -0.3325 | -0.5061 |  |  |  |  |
| 2-Methylphenol | 1.4357 | 1.0037 | 0.6409 | 0.3198 | 0.0329 | -0.2700 | -0.4919 | -0.6850 | -0.8634 |  |  |  |  |  |
| 2-Naphthol |  |  |  |  | 1.0909 | 0.7334 | 0.4538 | 0.2028 | -0.0205 | -0.2172 | -0.3775 | -0.5147 |  |  |
| 2-Nitroaniline |  |  |  |  |  | 0.5280 | 0.2679 | 0.0361 | -0.2167 | -0.3607 | -0.5079 | -0.5456 |  |  |
| 2-Nitrophenol |  | 1.1821 | 0.8225 | 0.5070 | 0.2287 | -0.0444 | -0.2590 | -0.4496 | -0.6244 | -0.8011 |  |  |  |  |
| 2-Nitropropane | 0.1358 | -0.1867 | -0.4793 | -0.7591 |  |  |  |  |  |  |  |  |  |  |
| 2-Nitrotoluene |  |  |  |  |  | 0.0382 | -0.1920 | -0.3520 | -0.5860 | -0.7214 | -0.8587 |  |  |  |
| 2-Nonanone | 1.5320 | 1.1314 | 0.7487 | 0.4154 | 0.1171 |  |  |  |  |  |  |  |  |  |
| 2-Octanone | 1.1587 | 0.4302 | 0.1123 | -0.1752 | -0.4289 |  |  |  |  |  |  |  |  |  |
| 2-Pentanone | -0.0039 | -0.3024 | -0.5944 | -0.8899 |  |  |  |  |  |  |  |  |  |  |
| 2-Phenylacetamide |  |  | 1.5969 | 1.1703 | 0.8126 | 0.4758 | 0.1976 | -0.0062 | -0.2282 | -0.4175 | -0.5562 |  |  |  |
| 2-Phenylethanol |  |  |  |  |  | -0.0889 | -0.3195 | -0.5236 | -0.7053 | -0.8736 |  |  |  |  |
| 2-Phenyl-1-propanol |  | 1.4261 | 1.0290 | 0.6815 | 0.3709 |  |  |  |  |  |  |  |  |  |
| 2-Undecanone |  |  | 1.3308 | 0.9434 | 0.6015 | 0.2495 | -0.0126 | -0.2533 | -0.4712 | -0.6696 |  |  |  |  |
| 2,3-Dimethylphenol |  | 1.3258 | 0.9295 | 0.5866 | 0.2886 |  |  |  |  |  |  |  |  |  |
| 2,4-Dimethylaniline |  |  | 0.9706 | 0.6298 | 0.3101 | 0.1142 |  |  |  |  |  |  |  |  |
| 2,4-Dinitroaniline |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 2,6-Dichloro-4-nitroaniline | |  |  |  |  |  |  | 0.5268 | 0.2884 | 0.0745 | -0.1323 | -0.2973 | -0.4631 | -0.6206 |
| 2,6-Dimethylphenol |  | 1.1085 | 0.7449 | 0.4233 | 0.1445 |  |  |  |  |  |  |  |  |  |
| 3-Aminopropyltriethoxysilane | |  |  |  |  | 0.1092 | -0.1577 | -0.3952 | -0.6013 | -0.8027 |  |  | -1.1461 |  |
| 3-Methylaniline |  |  |  |  |  | -0.1592 | -0.3845 | -0.5804 | -0.7514 | -0.9193 |  |  |  |  |
| 3-Methylbutanol | 0.2818 | -0.0784 | -0.3869 | -0.6974 | -0.9610 |  |  |  |  |  |  |  |  |  |
| 3-Methylphenol |  | 1.0846 | 0.7064 | 0.3728 | 0.0857 | -0.2177 | -0.4488 | -0.6456 | -0.8222 |  |  |  |  |  |
| 3-Nitroaniline |  |  |  |  |  | 0.6727 | 0.4007 | 0.1577 | -0.0632 | -0.2601 | -0.4220 | -0.5530 |  |  |
| 3-Phenylpropan-1-ol |  |  | 1.1695 | 0.8012 | 0.4878 |  |  |  |  |  |  |  |  |  |
| 3,3'-Dichlorobenzidine |  |  |  |  |  |  |  |  | 1.3282 | 1.0280 | 0.7161 | 0.4768 | 0.2578 | 0.0626 |
| 3,4-Dichloroanilne |  |  |  |  |  | 0.5569 | 0.2945 | 0.0659 | -0.1252 | -0.3105 |  |  |  |  |
| 3,5-Dimethylphenol |  | 1.2706 | 0.8919 | 0.5388 | 0.2358 | -0.0340 | -0.2682 | -0.4662 | -0.6454 |  |  |  |  |  |
| 4-acetylbiphenyl |  |  |  |  |  |  |  |  | 0.4290 | 0.1922 | -0.0198 | -0.2019 |  |  |
| 4-Bromoacetanilide |  |  |  |  |  | 1.0909 | 0.7599 | 0.4343 | 0.1943 |  |  |  |  |  |
| 4-Chloro-2-nitroaniline | |  |  |  |  | 0.9428 | 0.6358 | 0.3869 | 0.1041 |  |  |  |  |  |
| 4-Chloroaniline |  |  |  |  |  | 0.1004 | -0.1322 | -0.3360 | -0.5139 | -0.6808 |  |  |  |  |
| 4-Chlorophenol |  | 1.4236 | 1.0058 | 0.6519 | 0.3374 | 0.0445 | -0.1991 | -0.4083 | -0.5906 | -0.7597 |  |  |  |  |
| 4-Cyanophenol |  |  |  |  |  |  |  | -0.0466 | -0.2581 | -0.4734 |  |  |  |  |
| 4-Dimethylaminoazobenzene | |  |  |  |  |  |  | 1.0465 | 0.7906 | 0.5227 | 0.2674 | 0.0589 | -0.1422 | -0.3191 |
| 4-Fluoroaniline | 1.2335 | 0.8275 | 0.4943 | 0.1928 | -0.1801 |  |  | -0.7664 | -0.8984 | -1.0745 |  |  |  |  |
| 4-Hydroxybenzaldehyde | |  |  |  | 0.7232 | 0.4001 | 0.1344 | -0.1068 | -0.3160 | -0.5002 |  |  |  |  |
| 4-Hydroxybezylalcohol | |  |  |  |  | 0.3574 | 0.0982 | -0.1371 | -0.3401 | -0.5190 |  |  |  |  |
| 4-Methoxy-2-nitroaniline | |  |  |  |  | 1.0064 | 0.6871 | 0.3736 | 0.1467 |  |  |  |  |  |
| 4-Methoxybenzyl alcohol | |  | 1.3886 | 0.9539 | 0.6133 | 0.2631 | 0.0088 | -0.2398 | -0.4195 | -0.6091 | -0.7405 | -0.8722 | -0.9492 | -1.0217 |
| 4-Methylphenol |  | 1.0950 | 0.7145 | 0.3784 | 0.0882 | -0.2092 | -0.4465 | -0.6706 | -0.8240 |  |  |  |  |  |
| 4-Nitroaniline |  |  |  |  |  |  | 0.6460 | 0.3820 | 0.1474 | -0.0696 | -0.2650 | -0.4101 |  |  |
| 4-Nitrobenzyl alcohol |  |  |  |  |  | 0.7270 | 0.4436 | 0.1998 | -0.0204 | -0.2131 |  |  | -0.6762 | -0.7261 |
| 4-Nitrotoluene |  |  |  |  |  | 0.2058 | -0.0864 | -0.2940 | -0.4752 |  |  |  |  |  |
| 4-Phenylphenol |  |  |  |  |  | 1.1038 | 0.7860 | 0.5052 | 0.2558 | 0.0277 | -0.1669 | -0.3176 |  |  |
| 4,4'-Dibromobiphenyl |  |  |  |  |  |  |  | 0.9539 | 0.7092 | 0.4570 | 0.2184 | 0.0236 | -0.1685 | -0.3314 |
| 4,4'-Methylenedianiline | |  |  |  |  | 1.9131 | 1.5109 | 1.1019 | 0.8433 | 0.5707 |  |  |  |  |
| 8-Hydroxyquinoline |  |  |  |  |  |  |  | -0.0059 | -0.2305 | -0.4191 | -0.5683 | -0.6781 | -0.8386 | -0.8945 |
| Acenaphthene |  |  |  |  |  |  |  |  |  |  |  |  | -0.7087 | -0.7945 |
| Acenaphthylene |  |  |  |  |  | 0.6709 | 0.4289 | 0.1874 | -0.0285 | -0.2163 |  |  | -0.7273 | -0.8244 |
| Acetamide | 0.5172 | 0.1327 | -0.1723 |  |  |  |  |  |  |  |  |  |  |  |
| Acetoacetanilide | #NULL! | 1.0943 | 0.7144 | 0.3865 | 0.1044 | -0.1170 |  |  |  |  |  |  |  |  |
| Acetophenone | 1.4663 | 1.0564 | 0.7055 | 0.3947 | 0.1167 | -0.1830 | -0.4082 | -0.6040 | -0.7716 | -1.0268 |  |  |  |  |
| alpha-Isomethyl ionone | |  |  | 1.4354 | 1.0468 | 0.6365 | 0.3622 | 0.1097 | -0.1166 | -0.3199 | -0.4794 | -0.6217 | -0.8109 | -0.8641 |
| alpha-Pinene |  |  | 0.2832 | -0.0137 | -0.2505 | -0.4718 | -0.6805 | -1.0090 | -1.1616 | -1.2134 | -1.2867 |  |  |  |
| Amyl cinnamal |  |  |  | 1.8877 | 1.4522 | 0.9795 | 0.6769 | 0.4034 | 0.1503 | -0.0721 | -0.2880 | -0.4492 | -0.6197 | -0.6969 |
| Androsterone |  |  |  |  |  |  |  |  |  |  | 0.8034 | 0.5624 | 0.3308 | 0.1478 |
| Aniline | 1.1502 | 0.7688 | 0.4389 | 0.1455 | -0.1150 | -0.4052 | -0.6137 | -0.7966 |  |  |  |  |  |  |
| Anisole |  |  |  |  |  | -0.5854 | -0.8064 |  |  |  |  |  |  |  |
| Anthracene |  |  |  |  |  | 1.2437 | 0.9390 | 0.6782 | 0.4328 | 0.2089 | -0.0041 | -0.1731 | -0.3471 | -0.4506 |
| Anthraquinone |  |  |  |  |  |  |  |  | 0.6666 | 0.4218 | 0.1922 | 0.0029 | -0.1526 | -0.3331 |
| Azulene |  |  |  |  |  |  |  | -0.0687 | -0.2933 | -0.4686 | -0.6133 | -0.7533 | -0.8562 | -0.9486 |
| Benz[a]anthracene |  |  |  |  |  |  |  |  | 1.3088 | 1.0253 | 0.7265 | 0.4976 | 0.2802 | 0.0921 |
| Benzaldehyde | 1.0785 | 0.7073 | 0.3951 | 0.1067 | -0.1452 | -0.4433 | -0.6423 |  |  |  |  |  |  |  |
| Benzamide |  |  |  | 1.0557 | 0.7080 | 0.3705 | 0.1172 | -0.1114 | -0.3205 | -0.5044 | -0.6202 | -0.7370 |  |  |
| Benzene | -0.0669 | -0.3585 | -0.6384 | -0.8827 | -1.0015 |  |  |  |  |  |  |  |  |  |
| Benzenesulfonamide |  |  |  |  |  | 0.8495 | 0.5573 | 0.2962 | 0.0627 | -0.1459 | -0.3508 | -0.4896 | -0.6482 | -0.7153 |
| Benzidine |  |  |  |  |  |  |  |  | 0.8550 | 0.5891 | 0.3296 | 0.1214 | -0.0758 | -0.2421 |
| Benzodioxane |  | 1.3442 | 0.9693 | 0.6422 | 0.3514 |  |  |  |  |  |  |  |  |  |
| Benzo[a]pyrene |  |  |  |  |  |  |  |  | 1.7950 | 1.4875 | 1.1406 | 0.8923 | 0.6458 | 0.4329 |
| Benzo[e]pyrene |  |  |  |  |  |  |  |  | 1.7738 | 1.4654 | 1.1181 | 0.8655 | 0.6258 | 0.4124 |
| Benzo[ghi]perylene |  |  |  |  |  |  |  |  |  | 1.9534 | 1.5471 | 1.2145 | 0.9581 | 0.7232 |
| Benzonitrile | 1.1457 | 0.8361 | 0.5289 | 0.2313 | -0.0371 |  |  |  |  |  |  |  |  |  |
| Benzophenone |  |  |  |  |  | 0.9525 | 0.6564 | 0.3929 | 0.1554 | -0.0619 | -0.2392 | -0.4006 |  |  |
| Benzothiazole |  |  |  |  |  |  |  | -0.2216 | -0.4171 | -0.5837 | -0.6921 | -0.8874 | -0.9427 |  |
| Benzyl 2-ethylhexyl phthalate | |  |  |  |  |  |  | 1.7296 | 1.3653 | 1.0261 | 0.7153 | 0.4500 | 0.1641 | 0.1001 |
| Benzyl alcohol | 1.4001 | 0.9800 | 0.6204 | 0.3056 | 0.0278 | -0.2809 | -0.4954 | -0.6850 | -0.8499 |  |  |  |  |  |
| Benzyl cinnamate |  |  |  |  |  | 1.8458 | 1.4860 | 1.1754 | 0.8451 | 0.5941 | 0.2674 | 0.0565 | -0.1511 | -0.3047 |
| Benzyl salicylate |  |  |  |  |  | 1.4208 | 1.0928 | 0.8112 | 0.5185 | 0.2900 | 0.0222 | -0.1649 | -0.3528 | -0.4967 |
| beta-Pinene |  |  |  |  |  | -0.3607 | -0.5711 | -0.7734 | -0.9063 | -1.0639 | -1.2134 | -1.2867 |  |  |
| Biphenyl |  |  |  |  |  | 0.4612 | 0.2046 | -0.0183 | -0.2077 | -0.3921 |  |  |  |  |
| Borneol |  | 1.3242 | 0.9982 | 0.6562 | 0.3573 |  | -0.1774 | -0.3947 | -0.5699 | -0.7312 | -0.8110 | -0.9535 | -1.0926 |  |
| Bromobenzene | 0.9665 | 0.6119 | 0.3040 | 0.0158 | -0.2352 |  |  |  |  |  |  |  |  |  |
| Butan-1-ol | 0.0199 | -0.3406 | -0.6857 |  |  |  |  |  |  |  |  |  |  |  |
| n-Butylbenzene | 1.3709 | 0.9705 | 0.6213 | 0.3115 | 0.0359 |  |  |  |  |  |  |  |  |  |
| Butyl acetate | 0.5066 | 0.1529 | -0.1596 | -0.4538 | -0.7189 |  |  |  |  |  |  |  |  |  |
| Butyl benzoate |  |  |  | 1.1334 | 0.7865 |  |  |  |  |  |  |  |  |  |
| Butyl benzyl phthalate |  |  |  |  |  |  |  | 1.4337 | 1.1198 | 0.8124 | 0.5288 | 0.2901 | 0.0571 | -0.1241 |
| Butyl cyclohexyl phthalate | |  |  |  |  |  |  | 1.3893 | 0.9367 | 0.6560 | 0.3977 | 0.1630 | -0.0472 | -0.2267 |
| Butyl decyl phthalate |  |  |  |  |  |  | 1.1812 | 0.8378 | 0.5573 | 0.2929 | 0.0515 | -0.1481 | -0.3924 | -0.4983 |
| Butyl oleate |  |  |  |  |  |  |  |  | 1.1115 | 0.7951 | 0.5053 | 0.2510 | 0.0025 | -0.1766 |
| Butyl stearate |  |  |  |  |  |  |  | 1.5116 | 1.1526 | 0.8272 | 0.5280 | 0.2686 | 0.0300 | -0.1852 |
| Camphor |  |  | 0.9255 | 0.5921 | 0.3031 | 0.0101 | -0.2174 | -0.4331 | -0.5985 | -0.7641 | -0.8611 | -0.9737 |  | -1.2172 |
| Carbazole |  |  |  |  |  |  |  |  | 0.4771 | 0.2469 | 0.0194 | -0.1585 | -0.3082 | -0.4265 |
| Carvone |  |  | 1.1979 | 0.8345 | 0.5192 | 0.1794 | -0.0657 | -0.2955 | -0.4812 | -0.6603 | -0.7731 | -0.8965 | -1.0383 | -1.0741 |
| Chlorobenzene | 0.6401 | 0.3089 | 0.0203 | -0.2428 | -0.4771 |  |  |  |  |  |  |  |  |  |
| Chloroform | -0.2480 | -0.5775 |  |  |  |  |  |  |  |  |  |  |  |  |
| Cholestane |  |  |  |  |  |  |  |  |  |  | 1.1025 | 0.8260 | 0.5565 | 0.3405 |
| Cholesterol |  |  |  |  |  |  |  |  |  |  | 1.3651 | 1.0668 | 0.7784 | 0.5422 |
| Cholesteryl acetate |  |  |  |  |  |  |  |  |  |  | 1.4867 | 1.1737 | 0.8712 | 0.6162 |
| Chrysene |  |  |  |  |  |  |  |  | 1.3628 | 0.9848 | 0.7291 | 0.5003 | 0.2802 | 0.0927 |
| Cinnamyl alcohol |  |  |  |  |  | 0.3167 | 0.0664 | -0.1658 | -0.3687 | -0.5515 |  |  |  |  |
| Citronellal |  |  | 0.9142 | 0.5538 | 0.2465 | -0.0576 | -0.2986 | -0.5258 | -0.6786 | -0.8788 | -0.9752 | -1.0847 |  |  |
| Coumarin |  |  |  |  |  | 0.6102 | 0.3502 | 0.1164 | -0.0979 | -0.2889 | -0.4590 | -0.5635 | -0.7140 | -0.8142 |
| Cyclohexanol | 0.8429 | 0.4758 | 0.1570 | -0.1224 | -0.3863 |  |  |  |  |  |  |  |  |  |
| Cyclohexanone | 0.8225 | 0.4783 | 0.1748 | -0.1022 | -0.3482 |  |  |  |  |  |  |  |  |  |
| Cyclohexanone oxime |  |  |  |  |  | -0.2376 | -0.4576 | -0.6617 |  |  |  |  |  |  |
| Decamethyltetrasiloxane | |  | 1.2607 | 0.8725 | 0.5338 |  |  |  |  |  |  |  |  |  |
| Decan-1-ol | 1.1670 | 0.7974 | 0.4446 | 0.1330 | -0.1508 | 0.1881 | -0.0703 | -0.3011 | -0.5017 | -0.6885 |  |  |  |  |
| Decane |  |  |  |  |  | -0.4385 | -0.6599 |  |  |  |  |  |  |  |
| Di-(2-Methoxyethyl) phthalate | |  |  |  |  |  |  | 0.8910 | 0.6009 | 0.3367 | 0.1206 | -0.1088 | -0.3124 | -0.4520 |
| Di-2-ethylhexyl phthalate | |  |  |  |  |  |  |  | 1.5462 | 1.1916 | 0.7183 | 0.4600 | 0.1943 | -0.0131 |
| Di-n-Butyl phthalate |  |  |  |  | 1.2407 | 1.5894 | 1.2333 | 0.9207 | 0.6023 | 0.3513 | 0.0622 | -0.1344 | -0.3449 | -0.5183 |
| Di-n-Butyl succinate |  |  |  |  |  | 0.7825 | 0.4706 | 0.1762 | -0.0556 | -0.2710 | -0.4710 | -0.6335 | -0.7884 | -0.9292 |
| Di-n-Octyl phthalate |  |  |  |  |  |  |  |  |  | 1.4395 | 0.9368 | 0.6489 | 0.3739 | 0.1475 |
| Di(2-Ethoxyethyl) phthalate | |  |  |  |  |  |  | 1.0815 | 0.7677 | 0.4896 | 0.2443 | 0.0070 | -0.1951 | -0.3882 |
| Di(2-n-butoxyethyl) phthalate | |  |  |  |  |  |  |  |  | 0.9336 | 0.6367 | 0.3806 | 0.1311 | -0.0791 |
| Dibenzofuran |  |  |  |  |  | 0.7532 | 0.4833 | 0.2412 | 0.0158 | -0.1777 | -0.3367 | -0.4800 |  |  |
| Dibenzyl ether |  |  |  |  |  | 0.9976 | 0.6923 | 0.4263 | 0.1837 | -0.0408 | -0.2527 | -0.4187 | -0.5910 | -0.7317 |
| Dibenzylamine |  |  |  |  |  | 1.1426 | 0.8259 | 0.5461 | 0.2946 | 0.0629 | -0.1579 | -0.3258 |  |  |
| Dicyclohexyl phthalate | |  |  |  |  |  |  |  | 1.4446 | 1.1477 | 0.7326 | 0.4835 | 0.2379 | 0.0323 |
| Dicyclohexylamine |  |  |  |  |  | 0.5531 | 0.3368 | 0.0530 | -0.1686 | -0.3583 | -0.5207 |  |  |  |
| Diethyl adipate |  |  |  |  | 0.5410 |  |  | -0.1287 | -0.3205 | -0.5123 | -0.7182 | -0.8489 | -0.9271 | -1.1324 |
| Diethyl diethylmalonate | |  |  |  |  | 0.1899 | -0.0781 | -0.3013 | -0.4821 | -0.6504 | -0.8463 | -0.8981 | -1.0681 | -1.1255 |
| Diethyl phthalate |  |  |  |  |  |  |  | 0.2604 | 0.0251 | -0.1746 | -0.3820 | -0.5442 | -0.7246 | -0.7849 |
| Diethyl sebecate |  |  |  |  |  | 1.1799 | 0.9080 | 0.5449 | 0.2768 | 0.0311 | -0.2019 | -0.3877 | -0.5494 | -0.6995 |
| Dihydrocholesterol |  |  |  |  |  |  |  |  |  |  | 1.3697 | 1.0789 | 0.7918 | 0.5523 |
| Diisobutyl phthalate |  |  |  |  |  | 1.3977 | 1.0599 | 0.7523 | 0.4566 | 0.2021 | -0.0591 | -0.2531 | -0.4156 | -0.5556 |
| Dimethyl phthalate | 0.1255 | -0.1934 | -0.4892 | -0.7467 |  |  |  | 0.0424 | -0.1620 | -0.3934 | -0.5431 | -0.6247 | -0.7979 | -0.9078 |
| Diphenyl ether |  |  |  |  |  | 0.5320 | 0.2712 | 0.0024 | -0.1977 | -0.3970 |  |  | -0.7792 | -0.8914 |
| Diphenylamine |  |  |  |  |  |  |  |  |  |  | -0.2628 | -0.4253 |  |  |
| Dodecamethylcyclohexasiloxane | |  |  |  |  | 0.1918 | -0.0875 | -0.3330 | -0.5496 |  |  |  |  |  |
| Dodecamethylpentasiloxane | | 1.3634 | 1.0305 | 0.6729 | 0.3510 |  |  |  |  |  |  |  |  |  |
| Dodecane |  |  |  |  |  | 0.0367 | -0.2149 | -0.4374 | -0.6336 | -0.8198 | -0.9713 |  |  |  |
| Dodecanol | -0.3132 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Ethyl acetate |  | 1.3683 | 1.0058 | 0.6370 | 0.3374 |  |  |  |  |  |  |  |  |  |
| Ethyl benzoate | 0.6442 | 0.2799 | -0.0421 | -0.3585 | -0.5711 |  |  |  |  |  |  |  |  |  |
| Ethyl oleate |  |  |  |  |  |  | 1.5859 | 1.1627 | 0.8415 | 0.5456 | 0.2761 | 0.0493 | -0.1613 | -0.3770 |
| Eugenol |  |  |  |  |  | 0.3918 | 0.1273 | -0.1140 | -0.3188 | -0.5137 | -0.6517 | -0.7769 | -0.8487 | -0.9803 |
| Fluoranthene |  |  |  |  |  |  |  |  |  |  | 0.3136 | 0.1144 | -0.0605 | -0.2241 |
| Fluorene |  |  | 1.2599 | 0.8744 | 0.5386 | 0.8906 | 0.6086 | 0.3582 | 0.1336 | -0.0758 | -0.2628 | -0.4203 | -0.5773 | -0.6768 |
| Geranial |  |  | 1.2169 | 0.8327 | 0.4873 | 0.1929 | -0.0628 | -0.3028 | -0.5351 | -0.6790 | -0.7960 | -0.9308 |  |  |
| Geraniol |  |  |  |  |  | 0.1505 | -0.1058 | -0.3460 | -0.5329 | -0.7365 | -0.8346 | -0.9662 | -1.0741 | -1.0923 |
| Glycidoxypropyltrimethoxysilane | 0.8333 | 0.4734 | 0.1445 | -0.1553 | -0.4179 | 0.5551 | 0.2766 | -0.0046 | -0.2409 | -0.4498 |  |  | -0.9336 | -0.9537 |
| Heptanal | 0.0572 | -0.2709 | -0.5638 | -0.8375 |  |  |  |  |  |  |  |  |  |  |
| Hexachlorobenzene |  |  |  |  | 1.2947 | 1.0922 | 0.7942 | 0.5307 | 0.2944 | 0.0900 | -0.1245 | -0.2883 | -0.4196 | -0.5500 |
| Hexadecane |  |  |  |  |  | 0.8781 | 0.5605 | 0.2767 | 0.0230 | -0.2110 | -0.4231 | -0.5975 |  |  |
| Hexamethyldisiloxane | 0.4483 | 0.1073 | -0.2080 | -0.5395 |  |  |  |  |  |  |  |  |  |  |
| Hexanal | -0.3809 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Hexane | 0.8012 | 0.4139 | 0.0782 | -0.2236 | -0.5111 |  |  |  |  |  |  |  |  |  |
| Hexanol |  |  | 1.3237 | 0.9334 | 0.5804 |  |  |  |  |  |  |  |  |  |
| Hydroxycitronellal | 1.2973 | 0.9189 | 0.5926 | 0.3047 | 0.0502 | 0.2301 | -0.0318 | -0.2708 | -0.4812 | -0.6631 | -0.7814 | -0.9060 | -0.9062 | -0.9706 |
| Iodobenzene |  |  |  |  |  | -0.2144 | -0.4177 | -0.5996 | -0.7590 | -0.9215 |  |  |  |  |
| Isocyanatopropyltriethoxysilane | |  |  | 1.5779 | 1.1726 | 0.3288 | 0.0454 | -0.2120 | -0.4309 | -0.6296 |  |  | -1.0564 | -1.0987 |
| Lilial |  |  | 0.5639 | 0.2379 | -0.0258 | 0.7415 | 0.4570 | 0.1990 | -0.0402 | -0.2468 | -0.4234 | -0.5734 | -0.7087 | -0.8566 |
| Limonene |  | 1.1409 | 0.7600 | 0.4144 | 0.1200 | -0.2843 | -0.4929 | -0.7067 | -0.8786 | -1.0235 | -1.0805 | -1.1922 |  |  |
| Linalool |  |  |  |  |  | -0.1713 | -0.4036 | -0.6314 | -0.8066 | -0.9720 | -1.0483 | -1.1448 |  |  |
| Methacryloxypropyltrimethoxysilane | | |  |  |  | 0.4883 | 0.1936 | -0.0296 | -0.3034 | -0.5155 |  |  | -0.8746 | -0.9471 |
| Methyl abietate |  | 1.1527 | 0.7840 | 0.4641 | 0.1775 |  |  |  | 1.0955 | 0.8066 | 0.5395 | 0.3076 | 0.0759 | -0.1139 |
| Methyl benzoate | 0.1948 | -0.1140 | -0.3948 | -0.6433 | -0.8601 |  |  |  |  |  |  |  |  |  |
| Methyl Cyclohexane |  |  | 1.3677 | 0.9723 | 0.6230 |  |  |  |  |  |  |  |  |  |
| Methyl eugenol | 0.9051 | 0.5207 | 0.1884 | -0.1110 | -0.4690 | 0.4631 | 0.1818 | -0.0684 | -0.2881 | -0.4841 | -0.6277 | -0.7675 | -0.8710 | -1.0380 |
| Methyl hexanoate |  |  | 1.1104 | 0.7390 | 0.4103 |  |  |  |  |  |  |  |  |  |
| Methyl nonanoate |  | 1.1821 | 0.7934 | 0.4495 | 0.1436 |  |  |  |  |  |  |  | -1.1185 | -1.1395 |
| Methyltris(trimethylsiloxy)silane | |  | -0.0165 |  | -0.4443 |  |  |  |  |  |  |  |  |  |
| N,N-Diethyl-4-nitroaniline | |  |  |  |  | 1.4670 | 1.1062 | 0.7525 | 0.4989 | 0.2595 | 0.0582 |  |  |  |
| N,N-Diethylcarbanilide | |  |  |  |  |  | 1.1087 | 0.7584 | 0.4993 | 0.2629 | 0.0233 | -0.1508 | -0.3338 | -0.4654 |
| N,N-Diethyldodecamide | |  |  |  |  |  |  | 0.8114 | 0.5246 | 0.2649 | 0.0221 | -0.1800 | -0.3621 | -0.5098 |
| N,N-Dimethyl-4-nitroaniline | 1.5921 | 1.0278 | 0.7156 |  | 0.1545 | 1.1898 | 0.8638 | 0.5396 | 0.3055 | 0.0947 |  |  |  |  |
| N,N-Dimethylaniline |  |  |  |  |  | -0.0963 |  |  |  |  |  |  |  |  |
| N,N-Diphenyl-4-phenylenediamine | | 1.3343 | 0.9693 | 0.6498 | 0.3709 |  |  | 1.8317 | 1.5415 | 1.2158 | 0.9179 | 0.6540 | 0.4010 | 0.1941 |
| Naphthalene |  |  | 1.1722 | 0.7961 | 0.4711 | 0.0936 | -0.1349 | -0.3265 | -0.5017 | -0.6659 |  |  |  |  |
| Neral |  |  |  |  |  | 0.1375 | -0.1124 | -0.3484 | -0.4948 | -0.7156 | -0.7960 | -0.9308 |  |  |
| Nicotinamide |  |  |  |  |  |  |  | -0.0141 | -0.2182 | -0.3994 | -0.5541 |  | -0.8209 | -0.8954 |
| Nicotine | 1.5218 | 1.1162 | 0.7603 | 0.4546 | 0.1793 |  |  | -0.0784 | -0.2536 | -0.3950 | -0.5967 |  | -0.8451 | -0.8756 |
| Nitrobenzene | 1.5600 | 1.1261 | 0.7452 | 0.4132 | 0.1188 |  |  |  |  |  |  |  |  |  |
| Nonanal | 0.8379 | 0.4778 | 0.1491 | -0.1441 | -0.4177 |  |  |  |  |  |  |  |  |  |
| Octadecane |  |  |  |  |  | 1.2753 | 0.9241 | 0.6067 | 0.3249 | 0.0692 | -0.1780 | -0.3616 |  |  |
| Octaethylcyclotetrasiloxane | |  |  |  |  | 1.0967 | 0.7585 | 0.4592 | 0.1915 | -0.0520 |  |  |  |  |
| Octamethyltrisiloxane | 1.5112 | 1.0564 | 0.6722 | 0.3345 | 0.0393 |  |  |  |  |  |  |  |  |  |
| Octan-1-ol | 1.2740 | 0.8562 | 0.4847 | 0.1641 | -0.1162 |  |  |  |  |  |  |  |  |  |
| Octan-2-ol | 1.1961 | 0.7998 | 0.4421 | 0.1374 | -0.1427 |  |  |  |  |  |  |  |  |  |
| Octanal | 0.4587 | 0.1141 | -0.1890 | -0.4747 | -0.7253 |  |  |  |  |  |  |  |  |  |
| Octanophenone |  |  |  |  |  | 1.0327 | 0.7144 | 0.4322 | 0.1799 | -0.0535 | -0.2519 | -0.4253 | -0.5910 | -0.7153 |
| Octyltriethoxysilane |  |  |  |  |  | 0.5749 | 0.2691 |  |  |  |  |  | -0.9677 | -1.0987 |
| Pentachlorophenol | 0.3847 | 0.0454 | -0.2692 | -0.5725 | -0.8623 | 1.1628 | 0.8840 | 0.5791 | 0.3336 | 0.1116 | -0.0847 | -0.2392 |  |  |
| Pentan-1-ol | 0.1182 | -0.2300 | -0.5580 | -0.8663 |  |  |  |  |  |  |  |  |  |  |
| Pentan-2-ol | 0.1302 | -0.2152 | -0.5408 | -0.8440 |  |  |  |  |  |  |  |  |  |  |
| Perylene |  |  |  |  |  |  |  |  |  |  | 1.1454 | 0.8908 | 0.6416 | 0.4307 |
| Phenanthrene |  | 0.7032 | 0.3556 | 0.0546 | -0.2134 | 1.2354 | 0.9271 | 0.6547 | 0.4107 | 0.1888 | -0.0050 | -0.1812 | -0.3505 | -0.4934 |
| Phenol | 1.4042 | 0.9876 | 0.6305 | 0.3220 | 0.0387 | -0.4799 | -0.6877 |  |  |  |  |  |  |  |
| Phenylacetate |  |  |  |  |  | -0.2647 | -0.4850 | -0.6837 |  |  |  |  |  |  |
| Phenylcyclohexane |  |  |  |  |  | 0.3533 | 0.1070 | -0.1182 | -0.3154 | -0.4944 |  |  | -0.8277 | -0.9954 |
| Phthalimide |  |  |  |  |  | 0.6452 | 0.3686 | 0.1233 | -0.0976 | -0.2951 | -0.4704 | -0.5822 |  |  |
| Phthalonitrile |  |  |  |  |  | 0.3441 | 0.0975 | -0.1251 | -0.3267 | -0.5044 | -0.6635 | -0.7602 |  |  |
| Progesterone | 0.1145 | -0.2234 | -0.5465 | -0.8206 |  |  |  |  | 1.8856 | 1.5631 |  |  | 0.5781 | 0.3621 |
| Pyrene | 0.2791 | -0.0392 | -0.3289 | -0.5952 | -0.8429 |  |  |  |  |  | 0.3775 | 0.1813 |  |  |
| Pyridine |  |  |  |  |  |  |  |  | 1.8459 | 1.4977 |  |  |  |  |
| Quinine |  |  |  |  |  | 0.2131 | -0.0208 | -0.2326 | -0.4152 | -0.5847 | 1.1295 | 0.8356 | 0.5900 |  |
| Quinoline | 0.8033 | 0.4549 | 0.1513 | -0.1195 | -0.3690 |  |  |  |  |  |  |  | -0.9583 | -0.9803 |
| Styrene |  |  |  |  |  |  |  |  | 0.9480 | 0.6726 |  |  |  |  |
| p-Terphenyl |  | 1.3487 | 1.0157 | 0.6662 | 0.3360 | 0.0540 | -0.1841 | -0.4064 | -0.5714 | -0.7474 | 0.4022 | 0.1880 | -0.0198 | -0.2068 |
| Terpinen-4-ol |  |  |  |  |  |  |  |  |  |  | -0.8336 | -0.9718 | -1.1255 | -1.1680 |
| Tetraethylorthosilicate | -0.2161 | -0.5615 |  |  |  |  |  |  |  |  |  |  |  |  |
| Tetramethylorthosilicate | |  |  |  |  | -0.2561 |  |  |  |  |  |  |  |  |
| Thioacetamide | 0.3431 | 0.0267 | -0.2551 | -0.5066 | -0.7285 |  |  |  |  |  |  |  |  |  |
| Toluene |  |  |  |  |  | 1.1048 | 0.7950 | 0.5183 | 0.2708 | 0.0449 |  |  |  |  |
| Trans Stilbene |  |  |  |  |  |  |  | 0.6678 | 0.3747 | 0.1118 | -0.1600 | -0.3388 | -0.4874 | -0.6173 |
| Tri-n-Butyrin |  |  |  |  |  |  |  | 1.3602 | 1.0418 | 0.7571 | -0.1419 | -0.3365 | -0.5512 | -0.6695 |
| Tribenzylamine |  |  | 1.3131 | 0.9319 | 0.5862 |  |  |  |  |  | 0.4921 | 0.2633 | 0.0472 | -0.1438 |
| Triethylamine |  |  |  |  |  |  |  | 0.0014 | -0.1928 | -0.3689 |  |  |  |  |
| Triisopropanolamine |  |  |  |  |  |  |  |  |  |  | -0.5760 | -0.7127 | -0.8451 | -0.9380 |
| Tris(trimethylsiloxy)silane | |  |  |  |  |  |  | 1.8395 | 1.4707 | 1.1440 |  |  |  |  |
| Trimethoprin |  |  |  |  |  |  |  | 1.0540 | 0.6975 |  | 0.8423 | 0.5769 | 0.3272 | 0.1154 |
| Triphenylamine |  |  |  |  |  |  |  |  | 1.2507 | 0.9671 | 0.2088 | 0.0029 | -0.1879 | -0.3531 |
| Triphenylene |  |  |  |  |  |  |  | 1.0179 | 0.6646 | 0.4083 | 0.7354 | 0.5051 | 0.2878 | 0.0991 |
| Triphenylmethane | 1.5112 | 1.1075 | 0.7459 | 0.4085 | 0.1082 | -0.2069 | -0.4410 | -0.6567 |  |  | 0.1758 | -0.0321 | -0.1975 | -0.3770 |
| Undecane | 0.0337 | -0.2886 |  |  |  |  |  |  |  |  |  |  |  |  |
| Valeraldehyde |  |  |  |  |  | 0.4084 | 0.1482 | -0.0872 | -0.3023 | -0.4985 |  |  |  |  |
| Valerophenone |  |  |  |  |  | 0.4949 | 0.2283 | -0.0193 | -0.2200 | -0.4116 | -0.6495 | -0.7773 | -0.9271 | -0.9903 |
| Vanillin |  |  |  |  |  |  |  |  |  |  | -0.5563 | -0.6932 | -0.7700 | -0.8717 |

Table S-5

Retention factor database for Rtx-OPP (60 – 300 °C)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | log60 | log80 | log100 | log120 | log140 | log160 | log180 | log200 | log220 | log240 | log260 | log280 | log300 |
| 1-Acetonaphthone |  |  |  |  |  | 0.6977 | 0.4100 | 0.1503 | -0.0773 | -0.2714 | -0.4532 | -0.6277 |  |
| 1-Bromododecane |  |  |  |  |  | 0.3394 | 0.0750 | -0.1841 | -0.3978 | -0.5835 |  |  |  |
| 1-Bromonaphthalene |  |  |  |  |  | 0.3459 | 0.0952 | -0.1286 | -0.3266 | -0.5000 |  |  |  |
| 1-Chloronaphthalene |  |  |  |  |  | 0.1808 | -0.0590 | -0.2711 | -0.4511 | -0.6215 |  |  |  |
| 1-Hydroxyanthraquinone |  |  |  |  |  |  |  | 0.8445 |  | 0.3418 | 0.0964 | -0.1069 | -0.2682 |
| 1-Methylnaphthalene |  | 1.3490 | 0.9589 | 0.6170 | 0.3127 |  |  |  |  |  |  |  |  |
| 1-Naphthol |  |  | 1.4697 | 1.0754 | 0.7278 | 0.4166 | 0.1555 | -0.0800 | -0.2833 | -0.4596 | -0.6337 | -0.7723 |  |
| 1-Nitronaphthalene |  |  |  |  | 1.1345 | 0.7788 | 0.4963 | 0.2405 | 0.0143 | -0.1851 | -0.3573 | -0.5373 |  |
| 1-Nitropropane | 0.3781 | 0.0549 | -0.2283 | -0.4802 |  |  |  |  |  |  |  |  |  |
| 1-Nitropyrene |  |  |  |  |  |  |  | 1.5871 |  | 0.9725 | 0.6926 | 0.4719 | 0.2273 |
| 1-Phenylethanol | 1.0822 | 0.6938 | 0.3506 | 0.0497 | -0.2323 |  |  |  |  |  |  |  |  |
| 1-Phenyl-2-propanol | 1.3697 | 0.9472 | 0.5817 | 0.2591 | -0.0236 |  |  |  |  |  |  |  |  |
| 1,12-dodecanediol |  |  |  |  |  | 0.8726 | 0.5438 | 0.2583 | -0.0014 | -0.2111 |  |  | -0.7430 |
| 1,2-Dichlorobenzene | 0.9222 | 0.5607 | 0.2448 | -0.0316 | -0.2835 | -0.4755 | -0.6604 | -0.8212 | -0.9722 | -1.1056 |  |  |  |
| 1,2-Dimethylbenzene | 0.4398 | 0.1084 | -0.1918 | -0.4336 | -0.6738 | -0.8212 | -0.9811 | -1.1354 | -1.2578 |  |  |  |  |
| 1,2,4,5-Tetrachlorobenzene |  | 1.3557 | 0.9660 | 0.6231 | 0.3186 |  | -0.1911 | -0.3807 | -0.5908 | -0.7329 |  |  | -1.1570 |
| 1,2,4-Trichlorobenzene | 1.3393 | 0.9375 | 0.5874 | 0.2805 | 0.0034 |  |  |  |  |  |  |  |  |
| 1,2,5,6-Dibenzoanthracene |  |  |  |  |  |  |  | 2.1190 | 1.8673 | 1.4793 | 1.2311 |  |  |
| 1,3-Dibromobenzene | 1.3205 | 0.9236 | 0.5786 | 0.2753 | 0.0034 |  |  |  |  |  |  |  |  |
| 1,3-Dichlorobenzene | 0.8058 | 0.4530 | 0.1455 | -0.1258 | -0.3722 |  |  |  |  |  |  |  |  |
| 1,3-Dihydroxybenzene |  | 1.4123 | 0.9506 | 0.5805 | 0.2591 | 0.0276 | -0.2212 | -0.4334 | -0.5946 | -0.7872 |  |  | -1.2030 |
| 1,3-Dimethylbenzene | 0.3466 | 0.0197 | -0.2647 | -0.5173 | -0.7549 | -0.8913 | -1.0507 | -1.2146 | -1.3410 |  |  |  |  |
| 1,3-Dinitrobenzene |  |  |  | 1.4045 | 1.0376 | 0.6808 | 0.3982 | 0.1521 | -0.0671 | -0.2641 | -0.4394 | -0.6128 | -0.7630 |
| 1,3,5-Triethylbenzene |  |  |  |  |  | -0.3266 | -0.5364 | -0.7359 | -0.9067 | -1.0649 |  |  |  |
| 1,4-Dimethylbenzene | 0.3353 | 0.0099 | -0.2725 | -0.5233 | -0.7624 | -0.9067 | -1.0476 | -1.2146 | -1.3534 |  |  |  |  |
| 13-bis(trimethylsiloxy)-13-dimethylsilane | 0.6378 | 0.2326 | -0.1155 |  | -0.7144 |  |  |  |  |  |  |  |  |
| 1,3-Dichloro-1,1,3,3-tetramethyldisiloxane | 0.3600 | 0.0132 | -0.2817 | -0.5302 |  |  |  |  |  |  |  |  |  |
| 1,5-Dichloro-1,1,3,3,5,5-hexamethyltrisiloxane | 1.0368 | 0.6192 | 0.2584 | -0.0578 | -0.3496 |  |  |  |  |  |  |  |  |
| 1,5-Divinyl-1,1,3,3,5,5-hexamethyltrsiloxane | 0.8034 | 0.3554 | 0.0073 | -0.2932 | -0.5826 |  |  |  |  |  |  |  |  |
| 2-(1-naphthyl)ethanol |  |  |  |  |  | 0.7359 | 0.4446 | 0.1870 | -0.0480 | -0.2495 | -0.4419 | -0.6161 |  |
| 2-Acetonaphthone |  |  |  |  |  | 0.7795 | 0.4874 | 0.2240 | -0.0073 | -0.2152 | -0.4005 | -0.5764 | -0.7380 |
| 2-Chloroacetamide | 1.0221 | 0.6556 | 0.2445 | -0.0312 | -0.2972 |  |  |  |  |  |  |  |  |
| 2-Chloroaniline | 1.3310 | 0.9233 | 0.5705 | 0.2596 | -0.0192 |  |  |  |  |  |  |  |  |
| 2-Chlorophenol | 0.7886 | 0.4340 | 0.1260 | -0.1455 | -0.3922 |  |  |  |  |  |  |  |  |
| 2-Ethoxyethanol | 0.0048 | -0.3234 | -0.5797 |  |  |  |  |  |  |  |  |  |  |
| 2-Heptanone | 0.7334 | 0.3680 | 0.0483 | -0.2328 | -0.4919 |  |  |  |  |  |  |  |  |
| 2-Hexanone | 0.4249 | 0.0891 | -0.2059 | -0.4654 | -0.7080 |  |  |  |  |  |  |  |  |
| 2-Methoxycinnamaldehyde |  |  |  |  |  | 0.6830 | 0.3907 | 0.1208 | -0.1127 | -0.3097 | -0.4959 |  | -0.7580 |
| 2-Methoxyethanol | -0.2320 | -0.5285 |  |  |  |  |  |  |  |  |  |  |  |
| 2-Methoxynaphthalene |  |  |  |  |  | 0.3346 | 0.0852 | -0.1423 | -0.3441 | -0.5199 |  |  |  |
| 2-Methyl-2-butanol | -0.3326 |  |  |  |  |  |  |  |  |  |  |  |  |
| 2-Methylaniline |  |  |  |  |  | -0.3834 | -0.5715 | -0.7561 | -0.9023 | -1.0367 |  |  |  |
| 2-Methylbenzothiazole |  |  |  |  |  |  |  | -0.4406 | -0.6002 | -0.7301 | -0.9043 | -1.0878 | -1.1272 |
| 2-Methylbutanol | -0.0167 | -0.3284 | -0.5979 |  |  |  |  |  |  |  |  |  |  |
| 2-Methylnaphthalene |  |  |  |  |  | 0.0276 | -0.2097 | -0.4156 | -0.5838 | -0.7558 |  |  |  |
| 2-Methylphenol | 0.9958 | 0.6050 | 0.2669 | -0.0287 | -0.2962 | -0.5065 | -0.6993 | -0.8934 | -1.0250 | -1.1505 |  |  |  |
| 2-Methylpropanol | -0.4116 |  |  |  |  |  |  |  |  |  |  |  |  |
| 2-Naphthol |  |  | 1.5171 | 1.1183 | 0.7667 | 0.4449 | 0.1843 | -0.0468 | -0.2518 | -0.4271 | -0.6197 | -0.7817 |  |
| 2-Nitroaniline |  |  |  |  |  | 0.4420 | 0.1856 | -0.0360 | -0.2414 | -0.4271 | -0.5923 | -0.6906 |  |
| 2-Nitrophenol | 1.4856 | 1.0745 | 0.7134 | 0.3965 | 0.1124 | -0.1263 | -0.3455 | -0.5324 | -0.6751 | -0.7993 |  |  |  |
| 2-Nitropropane | 0.2643 | -0.0495 |  |  |  |  |  |  |  |  |  |  |  |
| 2-Nitrotoluene |  |  |  |  |  | -0.0564 | -0.2660 | -0.4738 | -0.6560 | -0.8068 | -0.9274 |  |  |
| 2-Nonanone | 1.3905 | 0.9555 | 0.5772 | 0.2470 | -0.0494 |  |  |  |  |  |  |  |  |
| 2-Octanone | 1.0638 | 0.6626 | 0.3126 | 0.0061 | -0.2703 |  |  |  |  |  |  |  |  |
| 2-Pentanone | 0.0730 | -0.2306 | -0.4958 |  |  |  |  |  |  |  |  |  |  |
| 2-Phenylacetamide |  |  | 1.5155 | 1.2325 | 0.8421 | 0.4679 | 0.2026 | -0.0432 | -0.2582 | -0.4181 | -0.6277 |  |  |
| 2-Phenylethanol |  |  |  |  |  | -0.3019 | -0.5022 | -0.7052 | -0.8558 | -0.9961 |  |  |  |
| 2-Phenyl-1-propanol |  |  |  | 0.3417 | 0.0496 |  |  |  |  |  |  |  |  |
| 2-Undecanone |  | 1.5195 | 1.0614 | 0.7003 | 0.3634 | 0.0654 | -0.1829 | -0.4070 | -0.6136 | -0.8082 |  | -1.1333 |  |
| 2,3-Dimethylphenol | 1.4633 | 0.9933 | 0.6175 | 0.2885 | -0.0014 |  |  |  |  |  |  |  |  |
| 2,4-Dinitroaniline |  |  |  |  |  |  | 1.2561 | 0.9416 | 0.6971 | 0.4077 | 0.1474 |  |  |
| 2,6-Dichloro-4-nitroaniline |  |  |  |  |  |  |  | 0.4030 | 0.1720 | -0.0468 | -0.2407 | -0.4068 |  |
| 2,6-Dimethylphenol | 1.2109 | 0.8018 | 0.4449 | 0.1365 | -0.1426 |  |  |  |  |  |  |  |  |
| 2468-tetramethyl-2468-tetravinylcyclo | 1.5313 | 1.0405 | 0.6170 | 0.2460 | -0.0779 |  |  |  |  |  |  |  |  |
| 3-Aminopropyltriethoxysilane | 1.7707 | 1.2391 | 0.7958 | 0.4110 | 0.0727 | -0.2118 | -0.4582 | -0.6570 | -0.8578 | -1.0247 |  |  |  |
| 3-Methylaniline |  |  |  |  |  | -0.3688 | -0.5726 | -0.7530 | -0.9113 | -1.0553 |  |  |  |
| 3-Methylbutanol | -0.0125 | -0.3233 | -0.5942 |  |  |  |  |  |  |  |  |  |  |
| 3-Methylphenol |  | 0.7069 | 0.3555 | 0.0457 | -0.2271 | -0.4511 | -0.6515 | -0.8085 | -0.9828 | -1.1505 |  |  |  |
| 3-Nitroaniline |  |  |  |  |  | 0.6267 | 0.3541 | 0.1085 | -0.1049 | -0.3027 | -0.4615 | -0.6430 |  |
| 3-Nitrotoluene |  |  |  |  |  | 0.0573 | -0.1632 | -0.3793 | -0.5634 | -0.6947 | -0.8549 |  |  |
| 3-Phenylpropan-1-ol |  | 1.2130 | 0.8179 | 0.4755 | 0.1708 |  |  |  |  |  |  |  |  |
| 3,3'-Dichlorobenzidine |  |  |  |  |  |  |  | 1.5087 | 1.1399 | 0.8406 | 0.5408 | 0.2906 | 0.0670 |
| 3,4-Dichloroanilne |  |  |  |  |  | 0.3417 | 0.0956 | -0.1335 | -0.3356 | -0.5072 |  |  |  |
| 3,5-Dimethylphenol | 1.3877 | 0.9536 | 0.5785 | 0.2491 | -0.0445 | -0.2811 | -0.4925 | -0.6470 | -0.7943 | -0.9319 |  |  |  |
| 4-acetylbiphenyl |  |  |  |  |  | 1.0929 | 0.7664 | 0.4706 | 0.2158 | -0.0076 | -0.2150 | -0.4170 |  |
| 4-Bromoacetanilide |  |  |  |  |  |  | 0.6920 | 0.3879 | #NULL! | -0.0573 | -0.2612 |  |  |
| 4-Chloro-2-nitroaniline |  |  |  |  |  |  | 0.4688 | 0.2035 | 0.0242 | -0.1631 | -0.3610 |  |  |
| 4-Chloroaniline |  |  |  |  |  | -0.0770 | -0.2859 | -0.4933 | -0.6408 | -0.8136 |  |  |  |
| 4-Chlorophenol | 1.4492 | 1.0155 | 0.6424 | 0.3182 | 0.0290 |  |  |  |  |  |  |  |  |
| 4-Cyanophenol |  |  |  | 1.1103 | 0.7534 |  |  |  |  |  |  |  |  |
| 4-Dimethylaminoazobenzene |  |  |  |  |  |  |  |  | 0.5090 | 0.2477 | -0.0021 | -0.2231 | -0.3859 |
| 4-Fluoroaniline | 1.0363 | 0.6489 | 0.3094 | 0.0167 | -0.2497 |  |  |  |  |  |  |  |  |
| 4-Hydroxybenzaldehyde |  |  | 1.3274 | 0.9358 | 0.5907 | 0.2610 | 0.0159 | -0.2137 | -0.3950 | -0.5495 |  |  |  |
| 4-Hydroxybezyl alcohol |  |  |  |  |  | 0.1704 | -0.0793 | -0.3008 | -0.4813 | -0.6226 |  |  |  |
| 4-Methoxy-2-nitroaniline |  |  |  |  |  |  | 0.5887 | 0.3084 | 0.0957 | -0.1196 | -0.3134 |  |  |
| 4-Methoxybenzyl alcohol |  | 1.4861 | 1.0565 | 0.6951 | 0.3705 | 0.0686 | -0.1744 | -0.3807 | -0.5963 | -0.7795 | -0.9732 |  |  |
| 4-Methylphenol | 1.0996 | 0.6951 | 0.3436 | 0.0367 | -0.2367 | -0.4535 | -0.6404 | -0.8212 | -1.0104 | -1.1165 |  |  |  |
| 4-Nitroaniline |  |  |  |  |  | 0.9133 | 0.6189 | 0.3530 | 0.1207 | -0.0858 | -0.2867 | -0.4518 |  |
| 4-Nitrobenzyl alcohol |  |  |  |  |  | 0.6574 | 0.3809 | 0.1355 | -0.0848 | -0.2680 |  |  | -0.7700 |
| 4-Nitrotoluene |  |  |  |  |  | 0.1098 | -0.1096 | -0.3190 | -0.4907 | -0.6430 |  |  |  |
| 4-Phenylphenol |  |  |  |  |  | 0.7404 | 0.4394 | 0.1747 | -0.0540 | -0.2698 | -0.4454 | -0.6351 |  |
| 4,4'-Dibromobiphenyl |  |  |  |  |  |  |  | 0.5479 | 0.2937 | 0.0846 | -0.1449 | -0.3502 | -0.4939 |
| 4,4'-Methylenedianiline |  |  |  |  |  |  | 1.2056 | 0.8726 | 0.6204 | 0.2919 | 0.0819 |  |  |
| 8-Hydroxyquinoline |  |  |  |  |  |  |  | -0.2522 | -0.4225 | -0.5650 | -0.7397 | -0.9188 | -1.0058 |
| Acenaphthene |  |  |  |  |  |  |  |  |  |  |  |  | -0.8950 |
| Acenaphthylene |  |  |  |  |  | 0.3492 | 0.0947 | -0.1275 | -0.3840 | -0.5045 |  |  | -0.9235 |
| Acetamide | 0.7664 | 0.3597 | 0.0211 | -0.2445 | -0.5025 |  |  |  |  |  |  |  |  |
| Acetophenone | 1.3466 | 0.9325 | 0.5751 | 0.2604 | -0.0211 | -0.2568 | -0.4855 | -0.6532 | -0.8175 | -0.9490 |  |  |  |
| alpha-Isomethyl ionone |  |  | 1.5571 | 1.1538 | 0.7908 |  |  |  |  |  | -0.6762 |  |  |
| alpha-Pinene | 0.4015 | 0.0872 | -0.1933 | -0.4469 | -0.6996 |  |  |  |  |  |  |  |  |
| Amyl cinnamal |  |  |  | 1.4805 | 1.0829 | 0.7057 | 0.4051 | 0.1272 | -0.1153 | -0.3181 | -0.5070 |  | -0.7760 |
| Androsterone |  |  |  |  |  |  | 1.9538 | 1.5227 | 1.1930 | 0.8879 | 0.6273 | 0.3864 |  |
| Aniline | 0.8999 | 0.5277 | 0.2017 | -0.0540 | -0.3611 | -0.5588 | -0.7208 | -0.8891 | -1.0462 |  |  |  |  |
| Anisole |  |  |  |  |  | -0.7359 | -0.8918 | -1.0493 |  |  |  |  |  |
| Anthracene |  |  |  |  |  | 0.9274 | 0.6287 | 0.3567 | 0.1224 | -0.0882 | -0.2826 |  |  |
| Anthraquinone |  |  |  |  |  |  |  |  |  | 0.2187 | 0.0037 | -0.2017 | -0.3607 |
| Azulene |  |  |  |  |  |  |  | -0.3766 | -0.5355 | -0.6593 | -0.8178 | -1.0020 | -1.0758 |
| Benz[a]anthracene |  |  |  |  |  |  |  | 1.2534 | 0.9418 | 0.6816 | 0.4117 | 0.1834 | -0.0176 |
| Benzaldehyde | 0.9466 | 0.5791 | 0.2595 | -0.0225 | -0.2776 | -0.4721 | -0.6591 | -0.8382 | -0.9746 | -1.1058 |  |  |  |
| Benzamide |  |  |  | 1.0528 | 0.7015 | 0.3664 | 0.1036 | -0.1175 | -0.3155 | -0.4853 | -0.6384 | -0.8037 |  |
| Benzene | -0.3578 | -0.6255 |  |  |  |  |  |  |  |  |  |  |  |
| Benzenesulfonamide |  |  |  |  |  | 0.8332 | 0.5405 | 0.2813 | 0.0537 | -0.1490 | -0.3338 | -0.5279 | -0.6260 |
| Benzidine |  |  |  |  |  |  |  |  |  | 0.3504 | 0.0935 | -0.1253 | -0.2977 |
| Benzo[a]pyrene |  |  |  |  |  |  |  | 1.7424 | 1.3942 | 1.1004 | 0.8081 | 0.5604 |  |
| Benzo[e]pyrene |  |  |  |  |  |  |  | 1.7279 | 1.3802 | 1.0869 | 0.7957 | 0.5474 | 0.3081 |
| Benzo[ghi]perylene |  |  |  |  |  |  |  | 2.1569 | 1.8005 | 1.4834 | 1.1636 | 0.9039 | 0.6259 |
| Benzonitrile | 1.1173 | 0.7456 | 0.4140 | 0.1234 | -0.1378 |  |  |  |  |  |  |  |  |
| Benzophenone |  |  |  |  |  | 0.7174 | 0.4284 | 0.1741 | -0.0632 | -0.2652 | -0.4568 | -0.6336 |  |
| Benzothiazole |  |  |  |  |  |  |  | -0.5059 | -0.6629 | -0.7627 | -0.9510 |  | -1.1513 |
| Benzyl 2-ethylhexyl phthalate |  |  |  |  |  |  | 1.7037 | 1.3639 | 1.0003 | 0.6762 | 0.3794 | 0.1179 | -0.0925 |
| Benzyl alcohol | 1.0505 | 0.6541 | 0.3176 | 0.0189 | -0.2505 | -0.4631 | -0.6490 | -0.8363 | -0.9964 | -1.1165 |  |  |  |
| Benzyl cinnamate |  |  |  |  |  | 1.6509 | 1.1777 | 0.9066 | 0.6118 | 0.3537 | 0.0131 |  | -0.4190 |
| Benzyl salicylate |  |  |  |  |  | 1.0703 | 0.7437 | 0.4246 | 0.1620 | -0.0727 | -0.2177 |  | -0.6080 |
| Bis(trimethylsiloxy)methylsilane | 0.0903 | -0.2623 | -0.5521 | -0.7867 | -1.1037 |  |  |  |  |  |  |  |  |
| Biphenyl |  |  |  |  |  | 0.0960 | -0.1520 | -0.3565 | -0.5254 | -0.7135 |  |  |  |
| Borneol | 1.3616 | 0.9502 | 0.5960 | 0.2857 | 0.0085 | -0.2314 | -0.4319 | -0.5970 | -0.7903 | -0.9107 |  |  |  |
| Bromobenzene | 0.5667 | 0.2355 | -0.0527 | -0.3068 | -0.5405 |  |  |  |  |  |  |  |  |
| Butan-1-ol | -0.2744 |  |  |  |  |  |  |  |  |  |  |  |  |
| n-Butylbenzene | 0.9220 | 0.5409 | 0.2087 | -0.0832 | -0.3454 |  |  |  |  |  |  |  |  |
| Butyl acetate | 0.3764 | 0.0303 | -0.2751 | -0.5449 |  |  |  |  |  |  |  |  |  |
| Butyl benzoate |  |  | 1.2183 | 0.8314 | 0.4906 |  |  |  |  |  |  |  |  |
| Butyl benzyl phthalate |  |  |  |  |  |  | 1.5524 | 1.1744 | 0.8384 | 0.5393 | 0.2719 | 0.0223 | -0.1770 |
| Butyl cyclohexyl phthalate |  |  |  |  |  | 1.6863 | 1.3639 | 1.0037 | 0.6816 | 0.3988 | 0.1327 | -0.0856 | -0.2747 |
| Butyl decyl phthalate |  |  |  |  |  | 1.3429 | 0.9491 | 0.6248 | 0.3379 | 0.0808 | -0.1541 | -0.3692 | -0.5185 |
| Butyl 2-ethylhexyl phthalate |  |  |  |  |  | 1.8051 | 1.3654 | 0.9996 | 0.6791 | 0.3772 | 0.1172 |  |  |
| Butyl octyl phthalate |  |  |  |  |  |  | 1.1465 | 0.8019 | 0.4968 |  |  |  |  |
| Butyl oleate |  |  |  |  |  | 1.8085 | 1.4640 | 0.9485 | 0.6165 | 0.3110 | 0.0528 | -0.1854 | -0.3830 |
| Butyl stearate |  |  |  |  |  |  | 1.3564 | 0.9821 | 0.6428 | 0.3358 | 0.0634 | -0.1942 | -0.3500 |
| Camphor | 1.5813 | 1.1602 | 0.7927 | 0.4702 | 0.1821 |  |  |  |  |  |  |  |  |
| Carbazole |  |  |  |  |  | 1.0664 | 0.7460 | 0.4678 | 0.2180 | -0.0006 | -0.2003 | -0.4023 | -0.5290 |
| Carvone |  | 1.4045 | 1.0090 | 0.6484 | 0.3360 | 0.0577 | -0.1719 | -0.3744 | -0.5634 | -0.7355 | -0.9644 |  |  |
| Chlorobenzene | 0.3059 | -0.0056 | -0.2778 | -0.5173 | -0.7427 |  |  |  |  |  |  |  |  |
| Cholestane |  |  |  |  |  |  | 1.8995 | 1.4668 | 1.1166 | 0.8064 | 0.5366 |  | 0.0650 |
| Cholesterol |  |  |  |  |  |  |  | 1.9276 | 1.5243 | 1.1728 | 0.8678 | 0.5939 | 0.3470 |
| Cholesteryl acetate |  |  |  |  |  |  |  |  | 1.7191 | 1.3552 | 1.0268 | 0.7285 | 0.4650 |
| Chrysene |  |  |  |  |  |  | 1.5549 | 1.1504 | 0.8270 | 0.5572 | 0.4153 | 0.1820 | -0.0040 |
| Cinnamyl alcohol |  | 1.4726 | 1.0666 | 0.6992 | 0.3722 | 0.0598 | -0.1786 | -0.3827 | -0.5558 | -0.7207 |  |  |  |
| Citronellal |  |  |  |  |  | -0.2217 | -0.4355 | -0.6194 | -0.8120 | -0.9544 |  |  |  |
| Coumarin |  |  |  |  |  | 0.6105 | 0.3430 | 0.1035 | -0.1042 | -0.3055 | -0.4766 | -0.6421 | -0.7760 |
| Cyclohexanol | 0.5117 | 0.1727 | -0.1207 | -0.3816 | -0.6235 |  |  |  |  |  |  |  |  |
| Cyclohexanone | 0.8284 | 0.4770 | 0.1700 | -0.1005 | -0.3483 |  |  |  |  |  |  |  |  |
| Cyclohexanone oxime |  |  |  |  |  | -0.4822 | -0.6747 | -0.8085 | -0.9470 | -1.0397 |  |  |  |
| Decaethylcyclopentasiloxane |  |  |  | 2.0080 | 1.5330 |  |  |  |  |  |  |  |  |
| Decamethylcyclopentasiloxane | 1.1535 | 0.7039 | 0.3169 | -0.0217 | -0.3242 |  |  |  |  |  |  |  |  |
| Decamethyltetrasiloxane | 0.8707 | 0.4475 | 0.0831 | -0.2333 | -0.5313 |  |  |  |  |  |  |  |  |
| Decan-1-ol |  | 1.2257 | 0.8147 | 0.4535 | 0.1341 | -0.1435 | -0.3698 | -0.5848 | -0.7625 | -0.9272 |  |  |  |
| Decane | 0.5836 | 0.2202 | -0.0990 | -0.3784 |  | -0.8287 | -0.9838 | -1.1431 | -1.3172 |  |  |  |  |
| Di-(2-Methoxyethyl) phthalate |  |  |  |  |  | 1.4843 | 1.0896 | 0.7513 | 0.4502 | 0.1796 | -0.0672 | -0.1776 | -0.4630 |
| Di-2-ethylhexyl phthalate |  |  |  |  |  |  | 1.7450 | 1.3718 | 1.0073 | 0.7382 | 0.3794 | 0.1233 | -0.1010 |
| Di-n-Butyl phthalate |  |  |  |  |  | 1.3454 | 0.9666 | 0.5986 | 0.3057 | 0.0528 |  |  | -0.5230 |
| Di-n-Butyl succinate |  |  |  |  | 1.1087 | 0.5784 | 0.2710 | -0.0099 | -0.2356 | -0.4449 | -0.6581 |  | -0.9680 |
| Di-n-Octyl phthalate |  |  |  |  |  |  |  | 1.6311 | 1.2406 | 0.8835 | 0.5719 | 0.2974 | 0.0540 |
| Di(2-Ethoxyethyl) phthalate |  |  |  |  |  | 1.7450 | 1.3483 | 0.8826 | 0.5567 | 0.2824 | 0.0223 | -0.2045 | -0.3880 |
| Di(2-n-butoxyethyl) phthalate |  |  |  |  |  |  |  | 1.3109 | 0.9496 | 0.6458 | 0.3345 | 0.0890 | -0.1260 |
| Dibenzofuran |  |  |  |  |  | 0.4304 | 0.1715 | -0.0632 | -0.2680 | -0.4532 | -0.6220 | -0.7829 |  |
| Dibenzyl ether |  |  |  |  |  | 0.5955 | 0.3035 | 0.0361 | -0.1897 | -0.3934 |  |  |  |
| Dibenzylamine |  |  |  |  |  |  | 0.3879 | 0.1239 | -0.1109 | -0.3146 | -0.5083 | -0.6877 |  |
| Dicyclohexyl phthalate |  |  |  |  |  |  | 1.7190 | 1.3725 | 1.0216 | 0.7144 | 0.4419 | 0.1894 | -0.0250 |
| Dicyclohexylamine |  |  | 1.0713 | 0.7267 | 0.3867 | 0.0702 | -0.1633 | -0.3821 | -0.5649 | -0.7356 | -0.8746 |  |  |
| Dicylcohexyl adipate |  |  |  |  |  | 1.8190 | 1.4389 | 1.0668 | 0.7438 | 0.4563 |  |  |  |
| Diethoxydimethylsilane | -0.1686 | -0.5005 | -0.7668 | -0.9671 |  |  |  |  |  |  |  |  |  |
| Diethyl adipate |  |  |  |  |  |  |  | -0.2444 | -0.4461 | -0.6284 | -0.8483 | -0.9868 | -1.1150 |
| Diethyl diethylmalonate |  |  |  |  | 0.3486 | 0.0332 |  | -0.4631 | -0.6419 | -0.8072 | -0.9727 |  | -1.2400 |
| Diethyl phthalate |  |  |  |  |  | 0.7479 | 0.4350 | 0.1371 | -0.0910 | -0.3141 | -0.5300 | -0.6819 | -0.7780 |
| Diethyl sebecate |  |  |  |  |  | 1.0167 | 0.6620 | 0.3312 | 0.0695 | -0.1747 | -0.3998 | -0.6112 | -0.7280 |
| Dihydrocholesterol |  |  |  |  |  |  |  | 1.9637 | 1.5388 | 1.2054 | 0.8945 | 0.6164 | 0.3750 |
| Diisobutyl phthalate |  |  |  |  |  | 1.1907 | 0.8334 | 0.5165 | 0.2337 | -0.0142 | -0.2387 | -0.4496 | -0.5990 |
| Dimethyl phthalate |  |  |  |  | 0.9791 | 0.5229 | 0.2390 | -0.0400 | -0.2497 | -0.4169 | -0.6723 | -0.7999 | -0.9350 |
| Dioxane | -0.0032 | -0.3092 | -0.5726 | -0.8069 |  |  |  |  |  |  |  |  |  |
| Diphenyl ether |  |  |  |  |  | 0.1224 | -0.1180 | -0.3356 | -0.5314 | -0.7222 |  |  | -1.0230 |
| Diphenylamine |  |  |  |  |  | 0.6871 | 0.2719 | 0.0231 | -0.2073 | -0.4038 | -0.5496 | -0.7495 |  |
| Dodecamethylcyclohexasiloxane | 1.7477 | 1.2378 | 0.7960 | 0.4083 | 0.0759 | -0.2229 | -0.4542 | -0.6672 | -0.8806 | -1.0649 |  |  |  |
| Dodecamethylpentasiloxane | 1.4872 | 0.9934 | 0.5684 | 0.1407 | -0.1301 |  |  |  |  |  |  |  |  |
| Dodecane | 1.2312 | 0.7889 | 0.4242 | 0.0949 | -0.2000 | -0.4535 | -0.6643 | -0.8459 | -1.0191 | -1.1546 |  |  |  |
| Ethyl acetate | -0.3110 |  |  |  |  |  |  |  |  |  |  |  |  |
| Ethyl benzoate | 1.5469 | 1.1026 | 0.7182 | 0.3820 | 0.0825 |  |  |  |  |  |  |  |  |
| Ethyl 2-methylbutyrate | 0.4239 | 0.0762 | -0.2236 | -0.4885 | -0.7379 |  |  |  |  |  |  |  |  |
| Ethyl oleate |  |  |  |  |  |  | 1.0746 | 0.6678 | 0.3842 | 0.1042 | -0.1405 | -0.3795 | -0.5260 |
| Ethyl propionate | -0.0140 | -0.3284 | -0.5997 |  |  |  |  |  |  |  |  |  |  |
| Ethylbenzene | 0.3011 | -0.0181 | -0.2987 | -0.5449 | -0.7804 |  |  |  |  |  |  |  |  |
| Eugenol |  |  |  |  |  | 0.1518 | -0.0975 | -0.3134 | -0.5021 | -0.6779 |  |  |  |
| Fluoranthene |  |  |  |  |  | 1.3874 | 1.0510 | 0.7513 | 0.4785 | 0.2427 | 0.0279 | -0.1782 | -0.3340 |
| Fluorene |  |  |  |  |  | 0.5321 | 0.2679 | 0.0255 | -0.1971 | -0.3784 | -0.5516 | -0.7206 | -0.8220 |
| Geranial |  |  | 1.1107 | 0.7454 | 0.4144 |  |  | -0.3466 | -0.5455 | -0.7104 |  |  |  |
| Geraniol | 1.7062 | 1.2282 | 0.8106 | 0.4605 | 0.1361 | -0.1375 | -0.3856 | -0.5541 | -0.7568 | -0.9408 |  |  |  |
| Glycidoxypropyltrimethoxysilane | |  |  |  |  | 0.3154 |  |  |  |  |  |  | -1.0710 |
| Heptanal | 0.7221 | 0.3588 | 0.0428 | -0.2351 | -0.4747 |  |  |  |  |  |  |  |  |
| Hexachlorobenzene |  |  |  |  |  | 0.6533 | 0.3779 | 0.1279 | -0.0895 | -0.2846 | -0.4621 | -0.6327 | -0.7890 |
| Hexadecane |  |  | 1.4180 | 0.9886 | 0.6111 | 0.2530 | -0.0283 | -0.2758 | -0.4986 | -0.6842 | -0.8911 | -1.0530 |  |
| Hexaethylcyclotrisiloxane | 1.8979 | 1.3845 | 0.9451 | 0.5563 | 0.2239 |  |  |  |  |  |  |  |  |
| Hexamethylcyclotetrasiloxane | -0.0618 | -0.4050 | -0.6882 | -0.9042 |  |  |  |  |  |  |  |  |  |
| Hexamethyldisilane | -0.3523 | -0.6458 | -0.8653 | -1.0202 |  |  |  |  |  |  |  |  |  |
| Hexamethyldisilathiane | 0.6252 | 0.2645 | -0.0468 | -0.2567 | -0.5838 |  |  |  |  |  |  |  |  |
| Hexamethyldisilazane | -0.0565 | -0.3758 | -0.6355 | -0.8404 | -1.1371 |  |  |  |  |  |  |  |  |
| Hexamethyldisiloxane | -0.6439 |  |  |  |  |  |  |  |  |  |  |  |  |
| Hexanal | 0.3760 | 0.0526 | -0.2291 |  |  |  |  |  |  |  |  |  |  |
| Hexanol | 0.4237 | 0.0787 | -0.2267 | -0.4885 |  |  |  |  |  |  |  |  |  |
| Hydroxycitronellal |  | 1.2513 | 0.8679 | 0.5137 |  |  |  | -0.4855 | -0.6459 | -0.8846 |  |  |  |
| Iodobenzene | 0.8615 | 0.5079 | 0.1999 | -0.0718 | -0.3183 | -0.5083 | -0.6855 | -0.8763 | -0.9936 | -1.0986 |  |  |  |
| Isocyanatopropyltriethoxysilane | | 1.6470 | 1.1770 | 0.7672 | 0.4033 | 0.0878 | -0.1765 | -0.4091 | -0.6159 | -0.7872 |  |  | -1.3140 |
| Lilial |  |  | 1.6293 | 1.1804 | 0.8386 | 0.4959 | 0.2149 | -0.0375 | -0.2546 | -0.4297 | -0.6624 |  |  |
| Limonene | 0.7073 | 0.3445 | 0.0397 | -0.2311 | -0.5034 | -0.7169 | -0.9102 |  |  |  |  |  |  |
| Linalool | 1.1624 | 0.7387 | 0.3595 | 0.0682 | -0.2272 | -0.4444 | -0.6774 | -0.8942 | -1.0643 |  |  |  |  |
| Methacryloxypropyltrimethoxysilane | |  | 1.3789 | 0.9337 | 0.5543 | 0.2107 | -0.0750 | -0.3242 | -0.5420 | -0.7326 |  |  | -1.1700 |
| Methyl abietate |  |  |  |  |  |  | 1.3138 | 0.9588 | 0.6532 | 0.3749 | 0.1207 | -0.1045 | -0.2890 |
| Methyl benzoate | 1.3002 | 0.8866 | 0.5275 | 0.2127 | -0.0693 |  |  |  |  |  |  |  |  |
| Methyl Cyclohexane | -0.2919 | -0.5591 |  |  |  |  |  |  |  |  |  |  |  |
| Methyl decanoate |  | 1.4780 | 1.0348 | 0.6530 | 0.3212 |  |  |  |  |  |  |  |  |
| Methyl eugenol |  | 1.7103 | 1.2350 | 0.8363 | 0.4780 | 0.1581 | -0.1049 | -0.3324 | -0.5224 | -0.7278 |  |  |  |
| Methyl hexanoate | 0.6833 | 0.3110 | -0.0133 | -0.2986 | -0.5590 |  |  |  |  |  |  |  |  |
| Methyl nonanoate | 1.6558 | 1.1793 | 0.7680 | 0.4082 | 0.0886 |  |  |  |  |  |  |  |  |
| Methyl octanoate | 1.3413 | 0.8997 | 0.5166 | 0.1825 | -0.1168 |  |  |  |  |  |  |  |  |
| Methylbis(trimethylsiloxy)vinylsilane | 0.4748 | 0.0941 | -0.2276 | -0.5031 | -0.7912 |  |  |  |  |  |  |  |  |
| Methyltriethoxysilane | 0.2965 |  |  |  |  |  |  |  |  |  |  |  |  |
| Methyltris(trimethylsiloxy)silane | 0.8037 | 0.3892 | 0.0336 | -0.2760 | -0.5672 |  |  |  |  |  |  |  |  |
| N-Methylacetamide | 1.0255 | 0.6458 | 0.2559 | -0.0428 | -0.3464 |  |  |  |  |  |  |  |  |
| N-Methylaniline |  |  |  |  |  |  |  |  |  |  |  |  |  |
| N,N-Diethyl-4-nitroaniline |  |  |  |  |  |  |  | 0.7903 |  | 0.2575 |  | -0.2535 | -0.4430 |
| N,N-Diethylcarbanilide |  |  |  |  |  |  | 0.7449 | 0.4296 | 0.1650 | -0.0583 | -0.2525 |  | -0.5740 |
| N,N-Diethyldodecamide |  |  |  |  |  |  | 0.9007 | 0.5451 | 0.2515 | 0.0039 | -0.2049 | -0.4124 |  |
| N,N-Dimethyl-4-nitroaniline |  |  |  |  |  |  | 0.8679 | 0.5710 | 0.3589 | 0.0935 | -0.1215 |  |  |
| N,N-Dimethylaniline |  |  | 0.4923 | 0.1815 |  | -0.2599 | -0.5226 |  |  |  |  |  |  |
| N,N-Diphenyl-4-phenylenediamine | |  |  |  |  |  |  | 1.4347 | 1.0900 | 0.7718 | 0.4962 | 0.2413 |  |
| Naphthalene | 1.4415 | 1.0338 | 0.6739 | 0.3565 | 0.0760 | -0.1699 | -0.3790 | -0.5690 | -0.7360 | -0.8845 |  |  |  |
| Neral |  | 1.4592 | 1.0351 | 0.6760 | 0.3538 |  | -0.3447 | -0.5455 | -0.7104 |  |  |  |  |
| Nicotinamide |  |  |  |  |  |  | 0.2554 | -0.0036 | -0.2132 | -0.3906 | -0.5592 | -0.7208 |  |
| Nicotine |  |  |  |  |  |  | -0.0795 | -0.3098 | -0.4814 | -0.6451 | -0.7924 |  | -1.1150 |
| Nitrobenzene | 1.4391 | 1.0352 | 0.6814 | 0.3729 | 0.0890 |  |  |  |  |  |  |  |  |
| Nonanal | 1.3660 | 0.9357 | 0.5629 | 0.3272 | -0.0543 |  |  |  |  |  |  |  |  |
| Nonane | 0.2605 | -0.0742 | -0.3672 | -0.6246 |  | -0.9828 | -1.1262 | -1.3115 |  |  |  |  |  |
| Octadecane |  |  |  |  |  | 0.6017 | 0.2861 | 0.0097 | -0.2441 | -0.4645 | -0.6571 | -0.8459 |  |
| Octaethylcyclotetrasiloxane |  |  | 1.7233 | 1.2570 | 0.8587 | 0.4937 | 0.1863 | -0.0737 | -0.3103 | -0.5144 |  |  |  |
| Octamethylcyclotetrasiloxane | 0.5751 | 0.1807 | -0.1558 | -0.4445 | -0.7397 |  |  |  |  |  |  |  |  |
| Octamethyltrisiloxane | 0.2150 | -0.1448 | -0.4458 | -0.6943 | -0.9975 |  |  |  |  |  |  |  |  |
| Octan-1-ol | 1.0805 | 0.6692 | 0.3101 | -0.0020 | -0.2843 |  |  |  |  |  |  |  |  |
| Octan-2-ol | 0.8440 | 0.4559 | 0.1186 | -0.1790 | -0.4519 |  | -0.8243 |  |  |  |  |  |  |
| Octanal | 1.0471 | 0.6517 | 0.3073 | 0.0066 | -0.2671 |  |  |  |  |  |  |  |  |
| Octanophenone |  |  |  |  |  | 0.7240 | 0.4188 | 0.1442 | -0.0947 | -0.3083 | -0.4905 | -0.6801 | -0.8400 |
| Octyltriethoxysilane |  | 1.6372 | 1.1436 | 0.7220 | 0.3573 | 0.0383 | -0.2363 |  |  |  |  |  | -1.2630 |
| Pentachlorophenol |  |  |  |  |  | 0.7683 | 0.4818 | 0.2235 | 0.0000 | -0.2026 | -0.3834 | -0.5589 |  |
| Pentan-1-ol | 0.0881 | -0.2314 |  |  |  |  |  |  |  |  |  |  |  |
| Pentan-2-ol | -0.1415 | -0.4466 |  |  |  |  |  |  |  |  |  |  |  |
| Pentan-3-ol | -0.1549 | -0.4562 |  |  |  |  |  |  |  |  |  |  |  |
| Perylene |  |  |  |  |  |  |  |  |  |  |  | 0.6145 | 0.3480 |
| Phenanthrene |  |  |  |  |  | 0.9117 | 0.6145 | 0.3416 | 0.1068 | -0.1018 | -0.2918 | -0.4748 | -0.5940 |
| Phenol | 0.8121 | 0.4356 | 0.1055 | -0.1790 | -0.4446 | -0.6445 | -0.8050 | -0.9936 | -0.9855 | -1.2835 |  |  |  |
| Phenyl acetate | 1.3425 | 0.9158 | 0.5452 | 0.2214 | -0.0673 | -0.3161 | -0.5297 | -0.7210 | -0.8891 | -1.0159 |  |  |  |
| Phenylcyclohexane | #NULL! | #NULL! | #NULL! | #NULL! | #NULL! | -0.0418 | -0.2638 | -0.4688 | -0.6595 | -0.8154 |  |  | -1.1320 |
| Phenylsilane | -0.0296 | -0.3331 | -0.5786 | -0.7790 | -1.0509 |  |  |  |  |  |  |  |  |
| Phenyltrimethoxysilane | 1.5493 | 1.0843 | 0.6807 | 0.3223 | 0.0114 |  |  |  |  |  |  |  |  |
| Phthalimide |  |  |  |  |  | 0.5647 | 0.2947 | 0.0530 | -0.1645 | -0.3401 | -0.5307 | -0.6848 |  |
| Phthalonitrile |  |  |  |  |  | 0.5735 | 0.3088 | 0.0735 | -0.1354 | -0.3257 | -0.4954 | -0.6310 |  |
| Progesterone |  |  |  |  |  |  |  |  | 1.6118 | 1.2790 |  |  |  |
| Propyl acetate | 0.0375 | -0.2804 | -0.5588 |  |  |  |  |  |  |  |  |  |  |
| Pyrene |  |  |  |  |  | 1.4538 | 1.1159 | 0.8116 | 0.5403 | 0.3035 | 0.0841 | -0.1223 |  |
| Pyridine | 0.1360 | -0.1655 | -0.4260 | -0.6626 |  |  |  |  |  |  |  |  |  |
| Quinine |  |  |  |  |  |  |  | 1.6470 | 1.3117 | 1.0239 |  | 0.5452 | 0.2916 |
| Quinoline |  |  |  |  |  | -0.0076 | -0.2349 | -0.4281 | -0.6046 | -0.7704 |  |  | -1.1359 |
| Styrene | 0.4676 | 0.1324 | -0.1609 | -0.4215 | -0.6617 |  |  |  |  |  |  |  |  |
| Terphenyl |  |  |  |  |  |  |  | 0.7920 | 0.4992 | 0.2658 | 0.0070 | -0.2134 | -0.3766 |
| Terpinen-4-ol | 1.3653 | 0.9465 | 0.5822 | 0.2643 | -0.0206 | -0.2637 | -0.4828 | -0.6391 | -0.8388 |  |  |  |  |
| Tetrahydofuran | -0.3613 | -0.6359 |  |  |  |  |  |  |  |  |  |  |  |
| Tetrakis(trimethylsiloxy)silane | 1.2727 | 0.8103 | 0.4108 | 0.0610 | -0.2463 |  |  |  |  |  |  |  |  |
| Thioacetamide |  |  | 0.9979 | 0.6358 | 0.3406 | -0.1321 | -0.3057 | -0.4377 |  |  |  |  |  |
| Toluene | 0.0953 | -0.2084 | -0.4749 | -0.7144 | -0.9626 |  |  |  |  |  |  |  |  |
| Trans Stilbene |  |  |  |  |  | 0.7412 | 0.4383 | 0.1754 | -0.0649 | -0.2793 | -0.4679 | -0.6634 | -0.7780 |
| Tri-n-Butyrin |  |  |  |  |  | 1.2217 | 0.8447 | 0.5095 | 0.2153 | -0.0431 | -0.2757 |  | -0.6400 |
| Tribenzylamine |  |  |  |  |  |  |  | 0.8773 | 0.5784 | 0.2999 | 0.0536 | -0.1664 |  |
| Tridecane | 1.5440 | 1.0730 | 0.6692 | 0.3162 | 0.0021 |  |  |  |  |  |  |  |  |
| Triisopropanolamine |  |  |  |  |  |  | 0.2300 | -0.0354 | -0.2359 | -0.4576 | -0.6431 | -0.8323 | -0.9430 |
| Tris(trimethylsiloxy)silane | 0.7306 | 0.3176 | 0.0333 | -0.2420 | -0.6352 |  |  |  |  |  |  |  |  |
| Trimethoprin |  |  |  |  |  |  |  | 1.5667 | 1.1940 | 0.8643 | 0.5697 | 0.3011 |  |
| Triphenylamine |  |  |  |  |  | 1.0748 | 0.7435 | 0.4421 | 0.1852 | -0.0459 | -0.2552 | -0.4502 | -0.5740 |
| Triphenylene |  |  |  |  |  |  |  | 1.2550 |  | 0.6826 | 0.4179 | 0.1886 | -0.0095 |
| Triphenylmethane |  |  |  |  |  | 1.0792 | 0.7434 | 0.4473 | 0.1743 | -0.0578 | -0.2685 | -0.4430 |  |
| Undecane | 0.9042 | 0.5082 | 0.1628 | -0.1417 | -0.4164 | -0.6241 | -0.8140 | -1.0076 | -1.1549 |  |  |  |  |
| Valeraldehyde | 0.0480 | -0.2500 | -0.5107 |  |  |  |  |  |  |  |  |  |  |
| Valerophenone |  |  |  |  |  | 0.2027 | -0.0488 | -0.2817 | -0.4760 | -0.6555 | -0.8272 | -0.9736 | -1.1090 |
| Vanillin |  |  | 1.5240 | 1.1299 | 0.7779 | 0.4430 | 0.1751 | -0.0582 | -0.2689 | -0.4498 | -0.6624 |  | -0.9390 |
| Vinylpentamethyldisiloxane | -0.2291 | -0.5563 | -0.8090 | -0.9913 |  |  |  |  |  |  |  |  |  |
| Vinyltrimethoxysilane |  |  |  | -0.7867 |  |  |  |  |  |  |  |  |  |

Table S-6

Retention factor database for DB-1701 (60 – 260 °C)

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | 60 | 80 | 100 | 120 | 140 | 160 | 180 | 200 | 220 | 240 | 260 |
| 1-Acetonaphthone |  |  |  |  |  | 1.382 | 1.078 | 0.8099 | 0.5726 | 0.3578 | 0.1843 |
| 1-Bromododecane |  |  |  |  |  | 1.0798 | 0.7832 | 0.5194 | 0.2885 | 0.0828 |  |
| 1-Bromonaphthalene |  |  |  | 1.0398 | 0.698 |  |  |  |  |  |  |
| 1-Bromonaphthalene |  |  |  |  |  | 1.0792 | 0.8206 | 0.5834 | 0.3722 | 0.1797 |  |
| 1-Chloronaphthalene |  |  |  |  |  |  | 0.6385 | 0.4146 | 0.215 | 0.0335 |  |
| 1-Hydroxyanthraquinone |  |  |  |  |  |  |  | 1.5603 | 1.2711 | 1.0129 | 0.7729 |
| 1-Methylnaphthalene |  | 1.4051 | 1.003 | 0.6456 | 0.3278 |  |  |  |  |  |  |
| 1-Naphthol |  |  |  | 1.5446 | 1.1167 |  |  |  |  |  |  |
| 1-Naphthol |  |  |  |  |  | 1.4482 | 1.1204 | 0.8318 | 0.5793 | 0.3499 | 0.1731 |
| 1-Nitronaphthalene |  |  |  |  |  | 1.4519 | 1.1514 | 0.8838 | 0.6475 | 0.4332 | 0.2371 |
| 1-Nitropropane | 0.1542 | -0.1815 | -0.4793 |  |  |  |  |  |  |  |  |
| 1-Nitropyrene |  |  |  |  |  |  |  | 2.3497 | 2.0051 | 1.6979 | 1.4213 |
| 1,12-dodecanediol |  |  |  |  |  | 1.7592 | 1.3842 | 1.0574 | 0.7709 | 0.5111 |  |
| 1,2-Dichlorobenzene | 0.9561 | 0.572 | 0.2426 | -0.0473 | -0.3118 |  |  |  |  |  |  |
| 1,2-Dichlorobenzene |  |  |  |  |  | 0.161 | -0.0335 | -0.2135 | -0.357 | -0.5042 |  |
| 1,2-Dimethylbenzene |  |  |  |  |  | -0.21 | -0.3941 | -0.5364 |  |  |  |
| 1,2,5,6-Dibenzoanthracene |  |  |  |  |  |  |  |  |  | 2.3331 | 2.0916 |
| 1,3-Dimethylbenzene |  |  |  |  |  | -0.2845 | -0.4554 | -0.599 |  |  |  |
| 1,3-Dinitrobenzene |  |  |  |  |  | 1.2707 | 0.9778 | 0.7143 | 0.4888 | 0.2821 | 0.106 |
| 1,3,5-Triethylbenzene |  |  |  |  |  | 0.3788 | 0.1467 | -0.062 | -0.2459 | -0.4073 |  |
| 1,4-Dimethylbenzene |  |  |  |  |  | -0.2815 | -0.451 | -0.5959 |  |  |  |
| 2-(1-naphthyl)ethanol |  |  |  |  |  | 1.596 | 1.271 | 0.9826 | 0.7277 | 0.4987 | 0.294 |
| 2-Acetonaphthone |  |  |  |  |  | 1.4598 | 1.1503 | 0.8779 | 0.6359 | 0.417 | 0.2236 |
| 2-Chloroacetamide | 0.9113 | 0.6014 | 0.2266 |  | -0.2846 |  |  |  |  |  |  |
| 2-Heptanone | 0.5346 | 0.1618 | -0.1635 | -0.4496 |  |  |  |  |  |  |  |
| 2-Hexanone | 0.1792 | -0.1063 | -0.4666 |  |  |  |  |  |  |  |  |
| 2-Methoxynaphthalene |  |  |  |  |  | 1.0604 | 0.7854 | 0.5414 | 0.3243 | 0.1322 |  |
| 2-Methylaniline |  |  |  |  |  | 0.3343 | 0.1185 | -0.0764 | -0.2556 | -0.4577 |  |
| 2-Methylbenzothiazole |  |  |  |  |  |  |  | 0.2442 | 0.0646 | -0.0833 | -0.2531 |
| 2-Methylnaphthalene |  |  |  |  |  | 0.7112 | 0.4678 | 0.2535 | 0.0618 | -0.1183 |  |
| 2-Methylphenol |  |  |  |  |  | 0.3561 | 0.1195 | -0.0885 | -0.2755 |  |  |
| 2-Naphthol |  |  |  | 1.5911 | 1.1605 |  |  |  |  |  |  |
| 2-Naphthol |  |  |  |  |  | 1.4914 | 1.1572 | 0.8685 | 0.6144 | 0.3854 | 0.1778 |
| 2-Nitroaniline |  |  |  |  |  | 1.2087 | 0.9178 | 0.6632 | 0.4369 | 0.233 | 0.0553 |
| 2-Nitrophenol |  |  |  |  |  | 0.4486 | 0.2302 | 0.0467 | -0.1327 | -0.2844 |  |
| 2-nitrotoluene |  |  |  |  |  | 0.5028 | 0.287 | 0.0836 | -0.079 | -0.2227 | -0.3724 |
| 2-Nonanone | 1.2311 | 0.7876 | 0.4064 | 0.0755 | -0.2252 |  |  |  |  |  |  |
| 2-Octanone | 0.8837 | 0.4762 | 0.1244 | -0.1797 | -0.4694 |  |  |  |  |  |  |
| 2-Pentanone | -0.1949 | -0.5036 |  |  |  |  |  |  |  |  |  |
| 2-Phenylacetamide |  |  |  | 1.2703 | 0.8731 |  |  |  |  |  |  |
| 2-Phenylacetamide |  |  |  |  |  | 1.2023 | 0.9093 | 0.646 | 0.4265 | 0.2242 | 0.0503 |
| 2-Phenylethanol |  |  |  |  |  | 0.4264 | 0.1934 | -0.0101 | -0.1815 | -0.3588 |  |
| 2-Undecanone | 1.9178 | 1.4009 | 0.9579 | 0.5732 | 0.2312 |  |  |  |  |  |  |
| 2-Undecanone |  |  |  |  |  | 0.6278 | 0.3685 | 0.1341 | -0.0622 | -0.2149 |  |
| 2,4-Dimethylaniline |  | 1.1581 | 0.743 |  | 0.0802 |  |  |  |  |  |  |
| 2,4-Dimethylaniline |  |  |  |  |  | 0.4931 | 0.2734 | 0.0468 |  |  |  |
| 2,4-Dinitroaniline |  |  |  |  |  |  |  |  |  | 1.0831 |  |
| 2,6-Dichloro-4-nitroaniline |  |  |  |  |  |  |  | 1.1351 | 0.8793 | 0.6447 | 0.4317 |
| 2,6-Dimethylphenol | 1.5596 | 1.0744 | 0.6598 | 0.3014 | -0.0108 |  |  |  |  |  |  |
| 3-Aminopropyltriethoxysilane |  |  | 0.8179 | 0.4173 | 0.1328 |  |  |  |  |  |  |
| 3-Aminopropyltriethoxysilane |  |  |  |  |  | 0.4675 | 0.2075 | -0.0229 | -0.2221 | -0.4014 |  |
| 3-Methylaniline |  |  |  |  |  | 0.3455 | 0.1224 | -0.0728 | -0.2473 | -0.4014 |  |
| 3-Methylphenol |  |  |  |  |  | 0.4313 | 0.1856 | -0.0311 | -0.2183 | -0.3842 |  |
| 3-Nitroaniline |  |  |  |  |  | 1.4467 | 1.1374 | 0.8613 | 0.6172 | 0.401 | 0.2258 |
| 3-Nitrotoluene |  |  |  |  |  | 0.5707 | 0.3759 | 0.1676 | -0.01 | -0.1706 | -0.3105 |
| 3,3'-Dichlorobenzidine |  |  |  |  |  |  |  | 2.4469 | 2.0582 | 1.7079 | 1.3963 |
| 3,4-Dichloroanilne |  |  |  |  |  | 1.2136 | 0.9196 | 0.6622 | 0.4341 | 0.233 |  |
| 3,5-Dimethylphenol |  | 1.4337 | 0.9659 | 0.563 | 0.2112 |  |  |  |  |  |  |
| 3,5-Dimethylphenol |  |  |  |  |  | 0.6125 | 0.3494 | 0.1162 | -0.0776 | -0.2598 |  |
| 4-acetylbiphenyl |  |  |  |  |  | 1.8356 | 1.4889 | 1.1818 | 0.9089 | 0.6639 | 0.4515 |
| 4-Bromoacetanilide |  |  |  |  |  | 1.9564 | 1.5711 | 1.2268 | 0.9497 |  |  |
| 4-Chloro-2-nitroaniline |  |  |  |  |  | 1.6216 | 1.2359 | 1.0089 | 0.7419 |  |  |
| 4-Chloroaniline |  |  |  |  |  | 0.6948 | 0.4455 | 0.2251 | 0.0363 | -0.1401 |  |
| 4-Chlorophenol |  |  |  |  |  | 0.8227 | 0.5369 | 0.296 | 0.084 | -0.1024 |  |
| 4-Dimethylaminoazobenzene |  |  |  |  |  |  |  | 1.6315 | 1.328 | 1.0525 | 0.8016 |
| 4-Hydroxybenzaldehyde |  |  |  |  |  |  |  |  |  | 0.252 |  |
| 4-Hydroxybezyl alcohol |  |  |  |  |  | 1.2152 | 0.8945 | 0.6161 | 0.3708 | 0.155 |  |
| 4-Methoxy-2-nitroaniline |  |  |  |  |  | 1.6574 | 1.3168 | 1.0238 | 0.7753 |  |  |
| 4-Methylphenol |  |  |  |  |  | 0.4287 | 0.1819 | -0.0319 | -0.2183 | -0.3899 |  |
| 4-Nitroaniline |  |  |  |  |  | 1.7923 | 1.4492 | 1.1462 | 0.8797 | 0.638 | 0.4195 |
| 4-Nitrotoluene |  |  |  |  |  | 0.667 | 0.4312 | 0.2195 | 0.0277 | -0.138 |  |
| 4-Phenylphenol |  |  |  |  |  | 1.8501 | 1.4792 | 1.1539 | 0.8688 | 0.6167 | 0.3908 |
| 4,4'-Dibromobiphenyl |  |  |  |  |  |  |  | 1.3704 | 1.0979 | 0.8464 | 0.6204 |
| 4,4'-Methylenedianiline |  |  |  |  |  |  | 2.1613 | 1.7726 | 1.4676 | 1.1616 |  |
| 8-Hydroxyquinoline |  |  |  |  |  |  |  | 0.3983 | 0.2165 | 0.0342 | -0.1217 |
| Acenaphthylene |  |  |  |  |  | 1.0606 | 0.7946 | 0.5565 | 0.3461 | 0.1577 |  |
| Acetamide | 0.8149 |  | -0.0123 |  |  |  |  |  |  |  |  |
| Acetoacetanilide |  | 0.5892 | 0.2491 | -0.0605 | -0.3144 |  |  |  |  |  |  |
| Acetophenone | 1.2411 | 0.8166 | 0.454 | 0.1356 | -0.152 |  |  |  |  |  | -0.5939 |
| Acetophenone |  |  |  |  |  | 0.3033 | 0.0868 | -0.1 | -0.264 | -0.4133 |  |
| Aniline | 1.0431 | 0.6262 | 0.2717 | -0.0161 | -0.3075 |  |  |  |  |  |  |
| Aniline |  |  |  |  |  | 0.1519 | -0.0522 | -0.2354 | -0.3937 |  |  |
| Anisole |  |  |  |  |  | -0.1214 | -0.3018 | -0.4635 |  |  |  |
| Anthracene |  |  |  |  |  | 1.7028 | 1.3836 | 1.1011 | 0.8469 | 0.6204 | 0.4124 |
| Anthraquinone |  |  |  |  |  |  |  | 1.4022 | 1.1348 | 0.8854 | 0.6608 |
| Azulene |  |  |  |  |  |  |  | 0.3107 |  | -0.0272 | -0.1734 |
| Benz[a]anthracene |  |  |  |  |  |  |  | 2.0584 | 1.7362 | 1.4451 | 1.1816 |
| Benzaldehyde | 0.8606 | 0.4762 | 0.1483 | -0.1436 | -0.4127 |  |  |  |  |  |  |
| Benzaldehyde |  |  |  |  |  | 0.0854 | -0.1076 | -0.2742 | -0.4193 | -0.5622 |  |
| Benzamide |  |  |  |  |  | 1.1174 | 0.8264 | 0.5691 | 0.3454 | 0.1396 | -0.0438 |
| Benzene | -0.4148 | -0.7277 |  |  |  |  |  |  |  |  |  |
| Benzenesulfonamide |  |  |  |  |  | 1.7409 | 1.3941 | 1.0868 | 0.8191 | 0.5793 | 0.3685 |
| Benzidine |  |  |  |  |  |  |  | 1.7954 | 1.3756 | 1.1814 | 0.9221 |
| Benzo[a]pyrene |  |  |  |  |  |  |  | 2.5898 | 2.2308 | 1.9089 | 1.6182 |
| Benzo[e]pyrene |  |  |  |  |  |  |  | 2.5732 | 2.2148 | 1.8938 | 1.6036 |
| Benzo[ghi]perylene |  |  |  |  |  |  |  |  | 2.6564 | 2.3084 | 1.9941 |
| Benzonitrile | 1.0135 | 0.6187 | 0.2758 | -0.0302 | -0.2905 |  |  |  |  |  |  |
| Benzophenone |  |  |  |  |  | 1.433 | 1.1247 | 0.8498 | 0.6065 | 0.3876 | 0.1906 |
| Benzothiazole |  |  |  |  |  |  |  | 0.1354 | 0.0145 | -0.1407 | -0.2821 |
| Benzyl 2-ethylhexyl phthalate |  |  |  |  |  |  |  |  | 1.7796 | 1.437 | 1.118 |
| Benzyl alcohol | 1.3091 | 0.8508 | 0.461 | 0.123 | -0.1779 |  |  |  |  |  |  |
| Benzyl alcohol |  |  |  |  |  | 0.2733 | 0.0521 | -0.1396 | -0.3152 | -0.4664 |  |
| Biphenyl |  |  | 1.177 | 0.7982 | 0.4617 |  |  |  |  |  |  |
| Biphenyl |  |  |  |  |  | 0.8492 | 0.587 | 0.3524 |  | -0.0198 |  |
| Bromobenzene | 0.5896 | 0.2374 | -0.0658 | -0.3358 |  |  |  |  |  |  |  |
| n-Butylbenzene | 0.9467 | 0.5464 | 0.204 | -0.0967 | -0.3809 |  |  |  |  |  |  |
| Butyl acetate | 0.1787 | -0.1666 | -0.4729 |  |  |  |  |  |  |  |  |
| Butyl benzoate |  | 1.6352 | 1.1834 | 0.7891 | 0.4407 |  |  |  |  |  |  |
| Butyl benzyl phthalate |  |  |  |  |  |  |  | 1.972 | 1.6173 | 1.2985 | 1.0176 |
| Butyl cyclohexyl phthalate |  |  |  |  |  |  | 2.0627 | 1.742 | 1.4164 | 1.1136 |  |
| Butyl decyl phthalate |  |  |  |  |  |  |  | 1.3178 | 1.0212 | 0.7484 | 0.4986 |
| Butyl 2-ethylhexyl phthalate |  |  |  |  |  |  |  |  | 1.7787 | 1.4331 | 1.122 |
| Butyl oleate |  |  |  |  |  |  |  | 1.7649 | 1.4171 | 1.0946 | 0.8097 |
| Butyl stearate |  |  |  |  |  |  |  | 1.7968 | 1.4407 | 1.1153 | 0.8195 |
| Camphor | 1.4463 | 1.0213 | 0.6336 | 0.3142 | 0.0221 |  |  |  |  |  |  |
| Carbazole |  |  |  |  |  |  | 1.6784 | 1.3569 | 1.0724 | 0.8181 | 0.5892 |
| Chlorobenzene | 0.2838 | -0.0474 | -0.3334 | -0.5874 |  |  |  |  |  |  |  |
| Cholestane |  |  |  |  |  |  |  |  |  | 1.6492 | 1.3523 |
| Cholesterol |  |  |  |  |  |  |  |  |  | 2.0782 | 1.7354 |
| Cholesteryl acetate |  |  |  |  |  |  |  |  |  | 2.1817 | 1.829 |
| Chrysene |  |  |  |  |  |  |  |  | 1.757 | 1.4581 | 1.1872 |
| Cinnamyl alcohol |  |  |  |  |  | 0.8585 | 0.5838 | 0.3491 | 0.1322 | -0.0534 |  |
| Coumarin |  |  |  |  |  | 1.216 | 0.9321 | 0.6827 | 0.4592 | 0.2601 | 0.0753 |
| Cyclohexanone | 0.6243 |  | -0.0448 | -0.3104 |  |  |  |  |  |  |  |
| Cyclohexanone oxime |  |  |  |  |  | 0.2375 | 0.0239 | -0.1838 | -0.3331 |  |  |
| Cyclopentanone | 0.2658 | -0.0669 | -0.3619 | -0.5607 |  |  |  |  |  |  |  |
| Decan-1-ol | 1.9204 | 1.3658 | 0.9297 | 0.5337 | 0.188 |  |  |  |  |  |  |
| Decan-1-ol |  |  |  |  |  | 0.5866 | 0.3228 | 0.0932 | -0.1063 | -0.2888 |  |
| Decane | 0.5972 | 0.2106 | -0.1278 | -0.4095 |  |  |  |  |  |  |  |
| Decane |  |  |  |  |  | -0.1941 | -0.3755 | -0.5499 |  |  |  |
| Di-(2-Methoxyethyl) phthalate |  |  |  |  |  |  |  | 1.4701 | 1.1599 | 0.8726 | 0.6177 |
| Di-2-ethylhexyl phthalate |  |  |  |  |  |  |  |  |  | 1.4319 | 1.1255 |
| Di-n-Butyl succinate |  |  |  |  |  |  |  | 0.5848 | 0.3487 | 0.1345 | -0.0727 |
| Di-n-Octyl phthalate |  |  |  |  |  |  |  |  |  | 1.6914 | 1.3596 |
| Di(2-Ethoxyethyl) phthalate |  |  |  |  |  |  |  | 1.6234 | 1.2955 | 0.9871 | 0.724 |
| Di(2-n-butoxyethyl) phthalate |  |  |  |  |  |  |  |  | 1.7649 | 1.4184 | 1.1125 |
| Dibenzofuran |  |  |  |  |  | 1.1615 | 0.8842 | 0.6366 | 0.417 | 0.2141 | 0.0406 |
| Dibenzyl ether |  |  |  |  |  | 1.4012 | 1.0871 | 0.8087 | 0.562 | 0.3402 | 0.1446 |
| Dibenzylamine |  |  |  |  |  | 1.542 | 1.2159 | 0.9282 | 0.6733 | 0.4451 | 0.2371 |
| Dicyclohexyl phthalate |  |  |  |  |  |  |  |  | 1.8068 | 1.4787 | 1.1918 |
| Dicyclohexylamine |  |  |  |  |  | 0.8059 | 0.5509 | 0.3224 | 0.1201 | -0.0595 |  |
| Dicylcohexyl adipate |  |  |  |  |  |  |  | 1.8039 | 1.4669 | 1.1637 |  |
| Diethyl adipate |  |  |  |  |  |  |  | 0.3039 | 0.0979 | -0.1079 |  |
| Diethyl diethylmalonate |  |  |  |  |  |  |  | 0.0901 | -0.0961 | -0.2536 | -0.4267 |
| Diethyl phthalate |  |  |  |  |  |  |  | 0.7585 | 0.5183 | 0.294 | 0.0756 |
| Diethyl sebecate |  |  |  |  |  |  |  | 0.9642 | 0.6891 | 0.4313 | 0.2034 |
| Dihydrocholesterol |  |  |  |  |  |  |  |  |  | 2.0818 | 1.749 |
| Diisobutyl phthalate |  |  |  |  |  | 1.8698 | 1.4949 | 1.1691 | 0.8775 | 0.6161 | 0.3863 |
| Dimethyl phthalate |  |  |  |  |  |  |  | 0.5569 | 0.3414 | 0.1338 | -0.057 |
| Dioxane | -0.1623 | -0.4858 |  |  |  |  |  |  |  |  |  |
| Diphenyl ether |  |  |  |  |  | 0.8831 | 0.6174 | 0.3835 | 0.174 | -0.0133 |  |
| Diphenylamine |  |  |  |  |  | 1.4521 | 1.1301 | 0.8465 | 0.5966 | 0.3728 | 0.1743 |
| Dodecamethylcyclohexasiloxane |  |  |  |  |  | 0.3307 | 0.0773 | -0.1481 | -0.3466 | -0.5117 |  |
| Dodecane | 1.286 | 0.8303 | 0.4352 | 0.0988 | -0.2181 |  |  |  |  |  |  |
| Dodecane |  |  |  |  |  | 0.2222 | -0.0078 | -0.2097 | -0.3824 |  | -0.7111 |
| Dodecanol |  |  | 1.4759 | 1.0261 | 0.634 |  |  |  |  |  |  |
| Ethyl benzoate | 1.4985 | 1.0415 | 0.6499 | 0.306 | 0.0007 |  |  |  |  |  |  |
| Ethyl oleate |  |  |  |  |  |  |  | 1.4696 | 1.1469 | 0.8507 | 0.5829 |
| Ethylbenzene | 0.2919 | -0.0482 | -0.3365 |  |  |  |  |  |  |  |  |
| Fluoranthene |  |  |  |  |  |  | 1.8349 | 1.5189 | 1.2348 | 0.9793 | 0.7469 |
| Fluorene |  |  |  |  |  | 1.2897 | 1.0008 | 0.744 | 0.516 | 0.3121 | 0.1257 |
| Glycidoxypropyltrimethoxysilane |  |  |  |  |  | 1.0011 | 0.6968 | 0.4288 | 0.1888 | -0.0181 |  |
| Heptanal | 0.5507 | 0.1787 | -0.1249 | -0.4022 |  |  |  |  |  |  |  |
| Heptane | -0.4728 |  |  |  |  |  |  |  |  |  |  |
| heptanol | 0.8774 | 0.4507 | 0.0889 | -0.2261 | -0.5203 |  |  |  |  |  |  |
| Hexachlorobenzene |  |  |  |  |  | 1.3921 | 1.0977 | 0.8354 | 0.6036 | 0.3939 | 0.2057 |
| Hexadecane |  |  | 1.5203 | 1.0706 | 0.6745 |  |  |  |  |  |  |
| Hexadecane |  |  |  |  |  | 1.0244 | 0.7175 | 0.4471 | 0.2117 | -0.0008 | -0.2025 |
| Hexamethylcyclotrisiloxane | -0.0352 | -0.3833 | -0.708 | -0.9601 |  |  |  |  |  |  |  |
| Hexamethyldisilane |  |  | -0.9753 | -1.1797 |  |  |  |  |  |  |  |
| Hexamethyldisiloxane | -0.5734 |  | -1.1342 |  |  |  |  |  |  |  |  |
| Hexanol | 0.5229 | 0.1297 | -0.2036 | -0.496 |  |  |  |  |  |  |  |
| Iodobenzene | 0.9549 | 0.572 | 0.2426 | -0.0473 | -0.3118 |  |  |  |  |  |  |
| Iodobenzene |  |  |  |  |  | 0.1771 | -0.0148 | -0.1878 | -0.3432 | -0.4849 |  |
| Isocyanatopropyltriethoxysilane |  |  |  |  |  | 0.7037 | 0.4211 | 0.1797 | -0.0388 | -0.2405 |  |
| Methacryloxypropyltrimethoxysilane |  |  |  |  |  | 0.884 | 0.5828 | 0.321 | 0.091 | -0.1173 |  |
| Methyl abietate |  |  |  |  |  |  |  | 1.7957 | 1.4705 | 1.1704 | 0.9041 |
| Methyl benzoate | 1.2483 | 0.8198 | 0.4528 | 0.1288 | -0.1591 |  |  |  |  |  |  |
| Methyl octanoate | 1.256 | 0.8035 | 0.4862 | 0.0826 | -0.2181 |  |  |  |  |  |  |
| N-Methylacetamide |  | 0.4673 | 0.0928 | -0.2183 |  |  |  |  |  |  |  |
| N-Methylaniline | 1.2753 | 0.8387 | 0.4666 | 0.1393 | -0.155 |  |  |  |  |  |  |
| N,N-Diethyl-4-nitroaniline |  |  |  |  |  |  | 1.7276 | 1.3987 | 1.1182 | 0.851 |  |
| N,N-Diethylcarbanilide |  |  |  |  |  |  | 1.5151 | 1.1944 | 0.9328 | 0.6695 | 0.4468 |
| N,N-Diethyldodecamide |  |  |  |  |  |  |  | 1.2372 | 0.9426 | 0.6695 | 0.4224 |
| N,N-Dimethyl-4-nitroaniline |  |  |  |  |  |  | 1.483 | 1.1789 | 0.9296 | 0.6695 |  |
| N,N-Dimethylaniline | 1.2015 | 0.7813 | 0.4214 | 0.1545 | -0.155 |  |  |  |  |  |  |
| N,N-Dimethylaniline |  |  |  |  |  | 0.2687 |  |  |  |  |  |
| N,N-Diphenyl-4-phenylenediamine |  |  |  |  |  |  |  |  |  | 1.7938 | 1.4709 |
| Naphthalene |  | 1.0491 | 0.6774 | 0.351 | 0.0545 |  |  |  |  |  |  |
| Naphthalene |  |  |  |  |  | 0.5039 | 0.2826 | 0.0838 | -0.0899 | -0.2487 |  |
| Nicotinamide |  |  |  |  |  |  |  | 0.743 | 0.515 | 0.2975 | 0.1009 |
| Nicotine |  |  |  |  |  |  |  | 0.3221 | 0.1379 | -0.0317 | -0.1821 |
| Octadecane |  |  |  |  |  | 1.4185 | 1.0726 | 0.7681 | 0.507 | 0.2648 | 0.0437 |
| Octaethylcyclotetrasiloxane |  |  |  |  |  | 1.2228 | 0.9006 |  | 0.3642 |  |  |
| Octan-1-ol | 1.2281 | 0.7656 | 0.3734 | 0.0335 | -0.2742 |  |  |  |  |  |  |
| Octan-2-ol |  |  |  |  |  |  |  |  |  |  |  |
| Octanal | 0.901 | 0.4946 | 0.1533 | -0.1486 | -0.422 |  |  |  |  |  |  |
| Octane | -0.1064 | -0.4402 |  |  |  |  |  |  |  |  |  |
| Octanophenone |  |  |  |  |  | 1.4338 | 1.1095 | 0.8225 | 0.5685 | 0.3363 | 0.1405 |
| Pentachlorophenol |  |  |  |  |  |  |  |  |  |  | 0.3902 |
| Pentan-1-ol | 0.1617 | -0.2014 | -0.5013 |  |  |  |  |  |  |  |  |
| Perylene |  |  |  |  |  |  |  |  |  |  | 1.6369 |
| Phenanthrene |  |  |  |  |  | 1.6859 | 1.3673 | 1.0854 | 0.8341 | 0.6084 | 0.4042 |
| Phenol |  | 0.9042 | 0.4837 | 0.1272 | -0.1942 |  |  |  |  |  |  |
| Phenol |  |  |  |  |  | 0.2481 | 0.0173 | -0.1866 | -0.3606 | -0.5193 |  |
| Phenyl acetate | 1.2237 | 0.7869 | 0.4842 | 0.0826 | -0.2181 |  |  |  |  |  |  |
| Phenyl acetate |  |  |  |  |  | 0.2467 | 0.0225 | -0.158 | -0.3348 | -0.4849 |  |
| Phenylcyclohexane |  |  |  |  |  | 0.6755 | 0.4321 | 0.2172 | 0.0299 | -0.1423 |  |
| Phthalimide |  |  |  |  |  | 1.3209 | 1.0135 | 0.7447 | 0.507 | 0.3014 | 0.1066 |
| Phthalonitrile |  |  |  |  |  | 1.137 | 0.8563 | 0.6112 | 0.3908 | 0.1957 | 0.0177 |
| Pyrene |  |  |  |  |  |  | 1.9091 | 1.5902 | 1.3043 | 1.0468 | 0.8145 |
| Pyridine | 0.0252 | -0.2891 | -0.5746 |  |  |  |  |  |  |  |  |
| Quinoline |  |  |  |  |  | 0.6673 | 0.4287 | 0.2209 | 0.0349 | -0.1348 |  |
| p-Terphenyl |  |  |  |  |  |  |  | 1.6596 | 1.3495 | 1.0689 | 0.8142 |
| Terpinen-4-ol |  | 1.0588 | 0.6974 | 0.3238 | -0.023 |  |  |  |  |  |  |
| n-Tetradecane | 1.9689 | 1.4382 | 0.9819 | 0.5869 | 0.235 |  |  |  |  |  |  |
| Tetrahydofuran | -0.5155 |  |  |  |  |  |  |  |  |  |  |
| Thioacetamide |  | 1.1308 | 0.7637 | 0.3981 | 0.089 |  |  |  |  |  |  |
| Thioacetamide |  |  |  |  |  | 0.4943 |  |  |  |  |  |
| Toluene | -0.0345 | -0.3533 |  |  |  |  |  |  |  |  |  |
| Trans Stilbene |  |  |  |  |  | 1.5318 | 1.211 | 0.9251 | 0.6715 | 0.4445 | 0.2525 |
| Tri-n-Butyrin |  |  |  |  |  | 1.8432 | 1.4547 | 1.1125 | 0.8124 | 0.5513 | 0.299 |
| Tribenzylamine |  |  |  |  |  |  |  | 1.7562 | 1.4364 | 1.1406 | 0.8738 |
| Tridecane | 1.6278 | 1.1348 | 0.71 | 0.3414 | 0.0098 |  |  |  |  |  |  |
| Triisopropanolamine |  |  |  |  |  |  |  | 0.6611 | 0.4232 | 0.2016 | -0.0045 |
| Triphenylamine |  |  |  |  |  | 2.0339 | 1.6665 | 1.3413 | 1.0531 | 0.7937 | 0.5658 |
| Triphenylene |  |  |  |  |  |  |  | 2.0697 | 1.6652 | 1.4548 | 1.1928 |
| Triphenylmethane |  |  |  |  |  |  | 1.6512 | 1.3241 | 1.0364 | 0.7766 | 0.5426 |
| Undecane | 0.9425 | 0.5222 | 0.1567 | -0.1516 | -0.457 |  |  |  |  |  | -0.8348 |
| Undecane |  |  |  |  |  | 0.0188 | -0.1921 | -0.3747 | -0.5402 | -0.6853 |  |
| Valerophenone |  |  |  |  |  | 0.8386 | 0.5724 | 0.3379 | 0.1311 | -0.0569 |  |
| Vinylpentamethyldisiloxane | -0.2296 | -0.5546 | -0.8691 | -1.1048 |  |  |  |  |  |  |  |
| Vinyltrimethoxysilane | 0.0712 | -0.2734 | -0.5864 | -0.8437 |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |

Table S-7

Retention factor database for DB-225 (60 – 240 °C)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | log60 | log80 | log100 | log120 | log140 | log160 | log180 | log200 | log220 | log240 |
| 1-Acetonaphthone |  |  |  |  |  | 0.9856 | 0.6631 | 0.3748 | 0.0899 | -0.0766 |
| 1-Bromododecane |  |  |  |  |  | 0.1521 | -0.1593 | -0.3986 |  |  |
| 1-Bromonaphthalene |  |  |  | 1.1714 | 0.8274 | 0.5455 | 0.2660 | 0.0193 | -0.1723 | -0.3957 |
| 1-Chloronaphthalene |  |  | 1.2894 | 0.9130 | 0.5922 | 0.3243 | 0.0653 | -0.1565 | -0.3371 | -0.5734 |
| 1-Hydroxyanthraquinone |  |  |  |  |  |  |  | 1.1694 | 0.8767 | 0.5794 |
| 1-Methylnaphthalene |  | 1.5209 | 1.1012 | 0.7354 | 0.4297 |  |  |  |  |  |
| 1-Naphthol |  |  |  |  | 1.5793 | 1.2081 | 0.8548 | 0.5403 | 0.2674 | 0.0323 |
| 1-Nitronaphthalene |  |  |  |  | 1.4021 | 1.0766 | 0.7587 | 0.4748 | 0.2351 | 0.0019 |
| 1-Nitropropane | 0.4155 | 0.0594 | -0.2514 | -0.5216 |  |  |  |  |  |  |
| 1-Nitropyrene |  |  |  |  |  |  |  | 2.0700 | 1.7084 | 1.3645 |
| 1,12-dodecanediol |  |  |  |  | 1.6939 | 1.3148 | 0.9386 | 0.5555 | 0.2618 | 0.0232 |
| 1,2-Dichlorobenzene | 0.9996 | 0.6113 | 0.2705 | -0.0272 | -0.2800 | #NULL! | -0.6828 | -0.8936 | -1.0531 |  |
| 1,2-Dimethylbenzene |  |  |  |  |  | -0.9307 | -1.1449 |  |  |  |
| 1,2,3,5-Tetrachlorobenzene |  | 1.3657 | 0.9624 | 0.6088 | 0.3407 | 0.0444 | -0.2100 | -0.4434 | -0.6655 | -0.8202 |
| 1,2,5,6-Dibenzoanthracene |  |  |  |  |  |  |  |  | 2.4714 | 2.0415 |
| 1,3-Dimethylbenzene | 0.2441 | -0.0975 | -0.3967 |  |  | -1.0414 | -1.2330 |  |  |  |
| 1,3-Dinitrobenzene |  |  |  |  |  | 1.0160 | 0.6968 | 0.4195 | 0.1825 | -0.0520 |
| 1,3,5-Triethylbenzene |  |  |  |  |  | -0.4500 | -0.6952 |  |  |  |
| 1,4-Dimethylbenzene |  |  |  |  |  | -1.0414 |  |  |  |  |
| 1,3-bis(trimethylsiloxy)-1,3-dimethylsilane | -0.1357 | -0.5557 | -0.8444 |  |  |  |  |  |  |  |
| 1,3-Dichloro-1,1,3,3-tetramethyldisiloxane | | -0.5667 |  |  |  |  |  |  |  |  |
| 1,5-Divinyl-1,1,3,3,5,5-hexamethyldisiloxane | 0.1156 | -0.2926 | -0.6021 | -0.8191 |  |  |  |  |  |  |
| 2-(1-naphthyl)ethanol |  |  |  |  |  | 1.2928 | 0.9386 | 0.6288 | 0.3463 | 0.0992 |
| 2-Acetonaphthone |  |  |  |  |  | 1.0581 | 0.7315 | 0.4458 | 0.1220 | -0.1052 |
| 2-Chloroacetamide |  |  | 0.7470 | 0.4089 | 0.1285 | -0.0747 |  |  |  |  |
| 2-Heptanone | 0.5445 | 0.1651 | -0.1647 | -0.4603 |  |  |  |  |  |  |
| 2-Hexanone | 0.2364 | -0.1086 | -0.4129 |  |  |  |  |  |  |  |
| 2-Methoxycinnamaldehyde |  |  | 2.1441 | 1.6663 | 1.2830 | 0.9591 | 0.6245 | 0.3307 | 0.0658 | -0.1472 |
| 2-Methoxynaphthalene |  |  |  |  |  | 0.5515 | 0.2684 | -0.0032 | -0.1957 | -0.4221 |
| 2-Methylaniline |  |  |  |  |  | -0.0950 | -0.3437 | -0.5590 | -0.7484 | -0.9594 |
| 2-Methylbenzothiazole |  |  |  |  |  |  |  | -0.2645 | -0.4320 | -0.6760 |
| 2-Methylnaphthalene |  |  |  |  |  | 0.1077 | -0.1484 | -0.3707 | -0.5502 | -0.7423 |
| 2-Methylphenol |  |  |  |  |  | -0.0222 | -0.2922 | -0.5300 | -0.7309 |  |
| 2-Naphthol |  |  |  |  | 1.6451 | 1.2744 | 0.9127 | 0.6008 | 0.3313 | 0.0739 |
| 2-Nitroaniline |  |  |  |  | 1.2954 | 0.9779 | 0.6619 | 0.3875 | 0.1533 | -0.0593 |
| 2-Nitrophenol |  |  |  |  |  | -0.0026 | -0.2006 | -0.4232 | -0.6410 |  |
| 2-Nitrotoluene |  |  |  |  |  | 0.0512 | -0.1763 | -0.4223 | -0.5362 | -0.7951 |
| 2-Nonanone | 1.1746 | 0.7303 | 0.3443 | 0.0219 | -0.2723 |  |  |  |  |  |
| 2-Octanone | 0.8638 | 0.4532 | 0.0858 | -0.1748 |  |  |  |  |  |  |
| 2-Pentanone | -0.1052 |  |  |  |  |  |  |  |  |  |
| 2-Phenylacetamide |  |  |  |  |  | 1.0841 | 0.7538 | 0.4527 | 0.2198 | -0.0523 |
| 2-Phenylethanol |  |  |  |  |  | 0.0101 | -0.2576 | -0.4868 | -0.6639 | -0.8555 |
| 2-Undecanone | 1.7894 | 1.2758 | 0.8336 | 0.4485 | 0.1366 | -0.1471 | -0.4201 | -0.6345 | -0.8400 | -1.0026 |
| 2,6-Dichloro-4-nitroaniline |  |  |  |  | 1.8435 | 1.5189 | 1.1684 | 0.8359 | 0.5496 | 0.2924 |
| 2,2,4,4,6,6-Hexamethylcyclotrisilazane | 0.7883 | 0.3617 | 0.0001 | -0.3046 | -0.5347 |  |  |  |  |  |
| 2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclosiloxane | 1.0676 | 0.5705 | 0.1461 | -0.2109 | -0.3630 |  |  |  |  |  |
| 3-Aminopropyltriethoxysilane |  |  |  |  |  | -0.2872 |  |  |  |  |
| 3-Methylaniline |  |  |  |  |  | -0.0810 | -0.3423 | -0.5636 | -0.7484 | -0.8942 |
| 3-Methylphenol |  |  | 1.1233 | 0.7221 | 0.3803 | 0.0832 | -0.1926 | -0.4387 |  |  |
| 3-Nitroaniline |  |  |  |  | 1.6365 | 1.2901 | 0.9476 | 0.6503 | 0.3769 | 0.1408 |
| 3-Nitrotoluene |  |  |  |  |  | 0.1495 | -0.0955 | -0.3318 | -0.4582 | -0.7104 |
| 3,4-Dichloroanilne |  |  |  |  |  | 0.9050 | 0.5844 | 0.3210 | 0.0977 | -0.1456 |
| 3,5-Dimethylphenol |  |  | 1.3204 | 0.8963 | 0.5316 | 0.2322 | -0.0526 | -0.2744 | -0.4510 | -0.6008 |
| 4-acetylbiphenyl |  |  |  |  |  | 1.4175 | 1.0534 | 0.7302 | 0.4394 | 0.1935 |
| 4-Bromoacetanilide |  |  |  |  |  | 1.8073 | 1.3845 | 1.0360 | 0.7132 | 0.4516 |
| 4-Chloro-2-nitroaniline |  |  |  |  |  | 1.3999 | 1.0208 | 0.7299 | 0.4469 | 0.2189 |
| 4-Chloroaniline |  |  |  |  |  | 0.3532 | 0.0979 | -0.1456 | -0.3193 | -0.5591 |
| 4-Chlorophenol |  |  |  |  |  | 0.5319 | 0.2398 | -0.0297 | -0.2922 | -0.3989 |
| 4-Cyanophenol |  |  |  |  |  | 1.0825 | 0.7520 | 0.4641 | 0.2155 |  |
| 4-Dimethylaminoazobenzene |  |  |  |  |  |  |  | 1.1266 | 0.8116 |  |
| 4-Fluoroaniline |  | 1.1102 | 0.7435 | 0.4020 | 0.1407 | -0.1605 | -0.4068 | -0.6419 | -0.8245 |  |
| 4-Hydroxybenzaldehyde |  |  |  |  |  |  |  |  | 0.2968 | 0.0612 |
| 4-Hydroxybezylalcohol |  |  |  | 1.9530 | 1.5246 | 1.1713 | 0.8028 | 0.4851 | 0.2168 | -0.0144 |
| 4-Methoxy-2-nitroaniline |  |  |  |  |  | 1.4684 | 1.0792 | 0.7748 | 0.4804 | 0.2399 |
| 4-Methoxybenzyl alcohol |  |  |  | 1.1698 | 0.8188 | 0.4945 | 0.1800 | -0.0834 | -0.3253 | -0.4834 |
| 4-Methylphenol |  |  |  |  |  | 0.0278 | -0.2067 | -0.4547 | -0.6437 |  |
| 4-Nitroaniline |  |  |  |  |  | 1.7498 | 1.3713 | 1.0353 | 0.7444 | 0.4846 |
| 4-Nitrobenzyl alcohol |  |  |  | 2.1178 |  |  |  |  |  |  |
| 4-Nitrotoluene |  |  |  |  |  | 0.2092 | -0.0135 | -0.2454 | -0.4456 | -0.6710 |
| 4-Phenylphenol |  |  |  |  |  | 1.6319 | 1.2318 | 0.8760 | 0.5721 | 0.2903 |
| 4,4'-Dibromobiphenyl |  |  |  |  |  |  |  | 0.8492 | 0.5702 | 0.2942 |
| 4,4'-Methylenedianiline |  |  |  |  |  |  | 2.0644 | 1.6360 | 1.2652 | 0.9608 |
| 8-Hydroxyquinoline |  |  |  |  |  |  |  | -0.0400 | -0.2192 | -0.4571 |
| Acenaphthylene |  |  |  |  |  | 0.5587 | 0.2718 | 0.0413 | -0.1978 | -0.3458 |
| Acetamide |  |  |  | 0.4930 | 0.1826 | -0.0821 | -0.4338 |  |  |  |
| Acetophenone |  | 1.0573 | 0.6747 | 0.3413 | 0.0810 | -0.1874 | -0.4184 | -0.6345 | -0.8059 |  |
| alpha-Isomethyl ionone |  |  | 1.4079 | 0.9679 | 0.6586 | 0.3441 | 0.0511 | -0.1966 | -0.4338 | -0.6020 |
| alpha-Pinene |  | -0.2970 | -0.4064 | -0.6589 |  |  |  |  |  |  |
| Amyl cinnamal |  |  | 2.0223 | 1.5213 | 1.1352 | 0.7981 | 0.4574 | 0.1738 | -0.1034 | -0.3060 |
| Androsterone |  |  |  |  |  |  |  | 1.9607 | 1.5917 | 1.2379 |
| Aniline | 1.4562 | 1.0061 | 0.6227 | 0.2814 | -0.0014 | -0.2400 | -0.4907 | -0.6996 | -0.8445 |  |
| Anisaldehyde |  |  | 1.3549 | 0.9650 | 0.6170 |  |  |  |  |  |
| Anisole |  |  |  |  |  | -0.7232 | -0.9374 | -1.1256 |  |  |
| Anthracene |  |  |  |  |  | 1.2206 | 0.8889 | 0.5961 | 0.3358 | 0.0977 |
| Anthraquinone |  |  |  |  |  |  |  | 1.0327 | 0.7486 | 0.4619 |
| Azulene |  |  |  |  |  |  |  | -0.2092 | -0.3697 | -0.5390 |
| Benz[a]anthracene |  |  |  |  |  |  |  | 1.6653 | 1.3285 | 1.0040 |
| Benzaldehyde | 1.1259 | 0.7149 | 0.3864 | 0.0924 | -0.2004 | -0.4073 | -0.6282 | -0.8161 |  |  |
| Benzamide |  |  |  |  | 1.3169 | 0.9811 | 0.6583 | 0.3756 | 0.1321 | -0.0630 |
| Benzene | -0.4016 |  |  |  |  |  |  |  |  |  |
| Benzenesulfonamide |  |  |  |  |  | 1.8188 | 1.4285 | 1.0618 | 0.7599 | 0.4873 |
| Benzo[a]pyrene |  |  |  |  |  |  |  | 2.2491 | 1.8680 | 1.5103 |
| Benzo[e]pyrene |  |  |  |  |  |  |  | 2.2365 | 1.8561 | 1.4985 |
| Benzo[ghi]perylene |  |  |  |  |  |  |  |  | 2.3321 | 1.9479 |
| Benzonitrile | 1.3105 | 0.8954 | 0.5350 | 0.2240 | -0.0576 |  |  |  |  |  |
| Benzophenone |  |  |  |  | 1.3130 | 0.9893 | 0.6624 | 0.3790 | 0.1196 | -0.1152 |
| Benzothiazole |  |  |  |  |  |  |  | -0.2854 | -0.4414 | -0.6491 |
| Benzyl 2-ethylhexyl phthalate |  |  |  |  |  | 2.3271 | 1.8331 | 1.3915 | 1.0095 | 0.6561 |
| Benzyl alcohol |  | 1.2357 | 0.8156 | 0.4619 | 0.1266 | -0.1203 | -0.3697 | -0.5926 | -0.7782 | -0.9256 |
| Benzyl cinnamate |  |  |  |  | 2.2223 | 1.8593 | 1.4385 | 1.0700 | 0.7388 | 0.4485 |
| Benzyl salicylate |  |  |  | 2.1251 | 1.6992 | 1.3567 | 0.9859 | 0.6637 | 0.3679 | 0.1354 |
| beta-Pinene |  | -0.0585 | -0.3678 | -0.6589 |  |  |  |  |  |  |
| Bis(trimethylsiloxy)methylsilane | -0.6031 |  |  |  |  |  |  |  |  |  |
| Borneol |  | 1.1691 | 0.7697 | 0.4233 | 0.1571 | -0.1447 | -0.4068 | -0.5980 | -0.8015 | -0.9337 |
| Bromobenzene | 0.6492 | 0.2897 | -0.0264 | -0.2945 |  |  |  |  |  |  |
| Butan-1-ol |  |  |  |  |  |  |  |  |  |  |
| Butyl acetate |  |  |  |  |  |  |  |  |  |  |
| Butyl benzyl phthalate |  |  |  |  |  |  | 1.9209 | 1.4945 | 1.1274 | 0.7852 |
| Butyl cyclohexyl phthalate |  |  |  |  |  | 2.0170 | 1.5777 | 1.1912 | 0.8462 | 0.5360 |
| Butyl decyl phthalate |  |  |  |  |  | 1.4974 | 1.0912 | 0.7855 | 0.4165 | 0.1459 |
| Butyl 2-ethylhexyl phthalate |  |  |  |  |  | 2.3242 | 1.8306 | 1.3952 | 1.0093 | 0.6156 |
| Butyl octyl phthalate |  |  |  |  |  | 1.6383 | 1.2238 | 0.8655 | 0.5389 |  |
| Butyl oleate |  |  |  |  |  | 1.5664 | 1.1223 | 0.7422 | 0.3919 | 0.1005 |
| Butyl stearate |  |  |  |  |  |  | 1.1018 | 0.7157 | 0.3626 | 0.0662 |
| Camphor | 1.5600 | 1.1190 | 0.7370 | 0.4030 | 0.0960 | -0.2094 | -0.4519 | -0.6677 | -0.8244 | -0.9529 |
| Carbazole |  |  |  |  |  | 1.7972 | 1.4107 | 1.0573 | 0.7678 | 0.4929 |
| Carvone |  | 1.4268 | 1.0165 | 0.6500 | 0.3644 | 0.0592 | -0.2100 | -0.4337 | -0.6513 | -0.7926 |
| Chlorobenzene | 0.3136 | -0.0270 | -0.3288 | -0.5827 |  |  |  |  |  |  |
| Cholestane |  |  |  |  |  | 2.1010 | 1.6700 | 1.2846 | 0.9405 |  |
| Cholesterol |  |  |  |  |  |  |  | 2.0863 | 1.6819 | 1.2901 |
| Cholesteryl acetate |  |  |  |  |  |  |  | 2.1004 | 1.6924 | 1.2895 |
| Chrysene |  |  |  |  |  |  | 2.0642 | 1.6741 | 1.3430 | 1.0172 |
| Cinnamyl alcohol |  |  | 1.6270 | 1.1835 | 0.7964 | 0.4980 | 0.2063 | -0.0352 | -0.2584 | -0.4466 |
| Citronellal |  | 0.9192 | 0.5502 | 0.2193 | -0.0467 | -0.3575 | -0.5137 | -0.8010 | -0.9953 |  |
| Coumarin |  |  |  |  |  | 0.9464 | 0.6412 | 0.3766 | 0.1387 | -0.0505 |
| Cycloheptanone | 1.2107 | 0.8032 | 0.4507 | 0.1631 | -0.1295 |  |  |  |  |  |
| Cyclohexanone oxime |  |  |  |  |  | -0.2095 | -0.3536 | -0.6002 | -0.7309 | -0.9653 |
| Cyclopentanone | 0.5023 | 0.1521 | -0.1446 | -0.4273 |  |  |  |  |  |  |
| Decaethylcyclopentasiloxane | #NULL! | 2.3897 | 1.7983 | 1.2869 | 0.8416 |  |  |  |  |  |
| Decamethylcyclopentasiloxane | 0.3111 | -0.1385 | -0.4922 | -0.7685 |  |  |  |  |  |  |
| Decamethyltetrasiloxane | 0.0241 | -0.4022 | -0.7276 |  |  |  |  |  |  |  |
| Decan-1-ol |  |  |  |  |  | -0.1262 | -0.4234 | -0.6600 | -0.8400 |  |
| Decane | 0.0361 | -0.3086 | -0.5259 |  |  |  |  |  |  |  |
| Di-(2-Methoxyethyl) phthalate |  |  |  |  |  | 1.9214 | 1.4849 | 1.0982 | 0.7538 | 0.4529 |
| Di-n-Butyl phthalate |  |  |  |  |  | 1.5030 | 1.0943 | 0.7410 | 0.4202 | 0.1547 |
| Di-n-Butyl succinate |  |  |  |  |  | 0.5279 | 0.1863 | -0.0920 | -0.3650 | -0.5853 |
| Di-n-Octyl phthalate |  |  |  |  |  |  | 2.1707 | 1.7100 | 1.2954 | 0.9168 |
| Di(2-Ethoxyethyl) phthalate |  |  |  |  |  |  | 1.5599 | 1.1636 | 0.8053 | 0.4909 |
| Di(2-n-butoxyethyl) phthalate |  |  |  |  |  |  | 2.0195 | 1.5747 | 1.1793 | 0.8133 |
| Dibenzofuran |  |  |  |  |  | 0.6212 | 0.3352 | 0.0838 | -0.1305 | -0.3574 |
| Dibenzyl ether |  |  | 2.0719 | 1.5662 | 1.1909 | 0.8496 | 0.5217 | 0.2332 | -0.0084 | -0.2489 |
| Dibenzylamine |  |  |  |  |  | 1.0086 | 0.6584 | 0.3586 | 0.1023 | -0.1483 |
| Dicyclohexyl phthalate |  |  |  |  |  |  | 2.0626 | 1.6406 | 1.2658 | 0.9245 |
| Dicyclohexylamine |  |  |  |  |  | -0.0236 | -0.2947 | -0.5240 | -0.7107 | -0.9096 |
| Dicylcohexyl adipate |  |  |  |  |  |  | 1.5162 | 1.1210 | 0.7862 | 0.4931 |
| Diethyl adipate |  |  |  |  |  | 0.2601 | -0.0537 | -0.3123 | -0.5605 | -0.7544 |
| Diethyl diethylmalonate |  |  |  |  |  | -0.1160 | -0.3982 | -0.6218 | -0.8405 |  |
| Diethyl phthalate |  |  |  | 1.6827 | 1.2756 | 0.9320 | 0.5835 | 0.2836 | 0.0009 | -0.2173 |
| Diethyl sebecate |  |  |  |  |  | 0.9683 | 0.5898 | 0.2711 | -0.0342 | -0.2389 |
| Dihydrocholesterol |  |  |  |  |  |  |  | 2.0728 | 1.6737 | 1.2834 |
| Diisobutyl phthalate |  |  |  |  |  | 1.2923 | 0.9055 | 0.5562 | 0.2671 | -0.0091 |
| Dimethyl phthalate |  |  |  |  |  | 0.7450 | 0.4208 | 0.1419 | -0.1302 | -0.3279 |
| Dioxane | 0.0012 | -0.3457 |  |  |  |  |  |  |  |  |
| Diphenyl ether |  | 1.7833 | 1.3236 | 0.9190 | 0.6019 | 0.2812 | -0.0013 | -0.2388 | -0.4547 | -0.6411 |
| Diphenylamine |  |  |  |  |  | 1.0618 | 0.7123 | 0.4096 | 0.0951 | -0.1036 |
| Dodecamethylpentasiloxane | 0.5848 | 0.0910 | -0.3146 | -0.6358 | -0.8240 |  |  |  |  |  |
| Dodecane | 0.6570 | 0.2423 | -0.0754 | -0.3382 |  |  |  |  |  |  |
| Dodecanol |  |  | 1.3752 | 0.9254 | 0.5418 |  |  |  |  |  |
| Ethyl oleate |  |  |  |  |  | 1.2592 | 0.8434 | 0.4893 | 0.1635 | -0.1052 |
| Ethylbenzene | 0.2398 | -0.0960 | -0.4129 |  |  |  |  |  |  |  |
| Eugenol |  | 1.9594 | 1.4815 | 1.0453 | 0.7106 | 0.3888 | 0.0917 | -0.1646 | -0.4056 | -0.5853 |
| Fluoranthene |  |  |  |  |  | 1.7590 | 1.3859 | 1.0501 | 0.7639 | 0.4960 |
| Fluorene |  |  |  |  |  | 0.7586 | 0.4534 | 0.1934 | -0.0230 | -0.2321 |
| Geranial |  | 1.5121 | 1.0798 | 0.6883 | 0.3875 | 0.0679 | -0.2118 | -0.4005 | -0.6675 | -0.8813 |
| Geraniol |  | 1.4583 | 0.9977 | 0.5974 | 0.2761 | -0.0500 | -0.3301 | -0.5539 | -0.8090 |  |
| Glycidoxypropyltrimethoxysilane |  | 2.1733 | 1.6330 | 1.1621 | 0.7467 | 0.4105 | 0.0908 | -0.1970 | -0.4281 | -0.6273 |
| Heptanal | 0.5604 | 0.1819 | -0.1021 | -0.3837 |  |  |  |  |  |  |
| heptanol | 0.9184 | 0.5018 | 0.1510 | -0.1498 | -0.4109 |  |  |  |  |  |
| Hexachlorobenzene |  |  | 1.8722 | 1.4169 | 1.0748 | 0.7715 | 0.4565 | 0.1909 | -0.0381 | -0.2512 |
| Hexadecane |  |  | 0.8719 | 0.4642 | 0.1153 | -0.1993 | -0.4201 | -0.6964 | -0.8226 | -1.0433 |
| Hexaethylcyclotrisiloxane | 1.3890 | 0.8790 | 0.4526 | 0.1097 | -0.1745 |  |  |  |  |  |
| Hexamethylcyclotrisiloxane | -0.5620 |  |  |  |  |  |  |  |  |  |
| Hexamethyldisilathiane | 0.2242 | -0.1317 | -0.4309 | -0.6584 |  |  |  |  |  |  |
| Hexanol | 0.6011 | 0.2173 | -0.1119 | -0.3649 |  |  |  |  |  |  |
| Hydroxycitronellal |  |  | 1.4205 | 0.9767 | 0.6262 | 0.2988 | -0.0061 | -0.2666 | -0.4963 | -0.6664 |
| Iodobenzene | 1.0593 | 0.6682 | 0.3271 | 0.0318 | -0.1734 | -0.4239 | -0.6337 | -0.8203 | -0.9739 |  |
| Isocyanatopropyltriethoxysilane |  |  |  |  |  | -0.0998 | -0.3895 | -0.6456 | -0.8226 |  |
| Lilial |  |  | 1.6924 | 1.2315 | 0.8726 | 0.5436 | 0.2278 | -0.0439 | -0.2983 | -0.4644 |
| Limonene |  | 0.1116 | -0.1467 | -0.3826 | -0.6409 | -0.8749 |  |  |  |  |
| Linalool |  | 0.8029 | 0.4251 | 0.0937 | -0.1849 | -0.5007 | -0.7301 | -0.9597 |  |  |
| Methacryloxypropyltrimethoxysilane | 2.4683 | 1.8671 | 1.3427 | 0.8962 | 0.4933 | 0.1744 | -0.1396 | -0.4215 | -0.5932 | -0.8149 |
| Methyl abietate |  |  |  |  |  | 1.9204 | 1.4919 | 1.1158 | 0.7803 | 0.4856 |
| Methyl eugenol |  |  |  | 1.0328 | 0.6761 | 0.3339 | 0.0218 | -0.2026 | -0.4420 | -0.6566 |
| Methyl nonanoate |  | 0.9182 | 0.5390 | 0.1920 | -0.0823 | -0.3974 | -0.6525 | -0.9191 |  |  |
| Methyl phenyl ether | 0.6990 | 0.3182 | -0.0104 | -0.3023 |  |  |  |  |  |  |
| Methylbis(trimethylsiloxy)vinylsilane | -0.1857 | -0.6054 |  |  |  |  |  |  |  |  |
| Methyltriethoxysilane | 0.0241 | -0.3611 | -0.6490 |  |  |  |  |  |  |  |
| Methyltris(trimethoxy)silane | -0.0446 | -0.4648 | -0.7671 |  |  |  |  |  |  |  |
| N-Methylacetamide |  |  | 0.5753 | 0.2574 | -0.0207 |  |  |  |  |  |
| N-Methylaniline | 1.5731 | 1.1138 | 0.7175 | 0.3676 | 0.0753 |  |  |  |  |  |
| N,N-Diethyl-4-nitroaniline |  |  |  |  |  |  |  | 0.9097 | 0.6173 | 0.4971 |
| N,N-Diethylcarbanilide |  |  |  | 2.0548 | 1.6261 | 1.2907 | 0.9223 | 0.6094 | 0.3233 | 0.1071 |
| N,N-Diethyldodecamide |  |  |  | 2.0392 | 1.5779 | 1.2000 | 0.8107 | 0.4737 | 0.1676 | -0.0768 |
| N,N-Dimethyl-4-nitroaniline |  |  |  |  |  |  |  |  |  | 0.3777 |
| N,N-Dimethylaniline | 1.3307 | 0.8954 | 0.5171 | 0.2063 | -0.1117 |  |  |  |  |  |
| N,N-Diphenyl-4-phenylenediamine | |  |  |  |  |  |  | 2.3185 | 1.8949 | 1.4802 |
| Naphthalene |  | 1.1887 | 0.7998 | 0.4637 | 0.1661 | -0.0659 | -0.3061 | -0.5130 | -0.6137 | -0.8330 |
| Neral |  | 1.3991 | 0.9867 | 0.6092 | 0.3177 | 0.0031 | -0.2691 | -0.4434 | -0.6675 | -0.8813 |
| Nicotinamide |  |  |  | 2.0408 | 1.6310 | 1.3051 | 0.9521 | 0.6405 | 0.3669 | 0.1354 |
| Nicotine |  | 1.6417 | 1.2203 | 0.8367 | 0.5335 | 0.2342 | -0.0395 | -0.2732 | -0.4889 | -0.6765 |
| Nitrobenzene |  | 1.1838 | 0.8008 | 0.4736 | 0.1788 |  |  |  |  |  |
| Nonane | -0.2820 | -0.5922 |  |  |  |  |  |  |  |  |
| Nonanol | 1.5647 | 1.0604 | 0.6444 | 0.2815 | -0.0351 |  |  |  |  |  |
| Octadecane |  |  |  |  |  | 0.1588 | -0.1547 | -0.4249 | -0.5688 | -0.9256 |
| Octaethylcyclotetrasiloxane | 2.1082 | 1.5269 | 1.0260 | 0.5620 | 0.2382 | -0.0833 | -0.3638 | -0.5660 | -0.7206 |  |
| Octamethylcyclotetrasiloxane | -0.1621 | -0.5593 | -0.8444 |  |  |  |  |  |  |  |
| Octan-1-ol | 1.2354 | 0.7827 | 0.3987 | 0.0649 | -0.2223 |  |  |  |  |  |
| Octan-2-ol |  | 0.4995 | 0.1436 | -0.1499 | -0.4017 | -0.7043 | -0.9451 |  |  |  |
| Octane | -0.6245 |  |  |  |  |  |  |  |  |  |
| Octanophenone |  |  |  |  |  | 0.7665 | 0.4293 | 0.1505 | -0.0901 | -0.3208 |
| Pentachlorophenol |  |  |  |  |  | 1.3717 | 1.0073 | 0.6852 | 0.4088 | 0.1617 |
| Pentan-1-ol | 0.2748 | -0.0718 | -0.3455 | -0.5827 |  |  |  |  |  |  |
| Perylene |  |  |  |  |  |  |  | 2.2986 | 1.9272 | 1.5410 |
| Phenanthrene |  |  |  |  |  | 1.2136 | 0.8804 | 0.5893 | 0.3346 | 0.0956 |
| Phenol |  | 1.3529 | 0.9129 | 0.5351 | 0.2189 | -0.0689 | -0.3367 | -0.5544 | -0.7557 |  |
| Phenylcyclohexane |  | 1.2627 | 0.8631 | 0.5178 | 0.2416 | -0.0749 | -0.3232 | -0.5453 | -0.7173 | -0.8744 |
| Phenylsilane | -0.1120 | -0.4448 | -0.6768 |  |  |  |  |  |  |  |
| Phenyltrimethoxysilane | 1.6490 | 1.1796 | 0.7273 | 0.3620 | 0.0367 |  |  |  |  |  |
| Phthalimide |  |  |  |  |  | 1.1673 | 0.8182 | 0.5333 | 0.2783 | 0.0275 |
| Phthalonitrile |  |  |  |  |  | 0.9430 | 0.6399 | 0.3764 | 0.1387 | -0.0637 |
| Progesterone |  |  |  |  |  |  |  |  | 2.0680 | 1.6620 |
| Pyrene |  |  |  |  |  | 1.8464 | 1.4720 | 1.1342 | 0.8444 | 0.5784 |
| Pyridine | 0.2550 | -0.0853 | -0.3688 | -0.5981 |  |  |  |  |  |  |
| Quinine |  |  |  |  |  |  |  |  | 1.8792 | 1.4924 |
| Quinoline |  |  |  |  |  | 0.1972 | -0.0621 | -0.2979 | -0.4849 | -0.6555 |
| Styrene |  | 0.1143 | -0.1538 | -0.3697 | -0.5997 | -0.7770 | -0.9163 |  |  |  |
| p-Terphenyl |  |  |  |  |  |  | 1.4127 | 1.0749 | 0.7473 |  |
| Terpinen-4-ol | 1.5300 | 1.0580 | 0.6480 | 0.3000 | -0.0230 | -0.2703 | -0.5182 | -0.7203 | -0.9307 |  |
| n-Tetradecane | 1.2697 | 0.7913 | 0.4038 | 0.0475 | -0.2502 |  |  |  |  |  |
| Tetraethylorthosilicate | 0.4138 | -0.0103 | -0.3382 | -0.6061 | -0.7853 |  |  |  |  |  |
| Tetrahydofuran | -0.4857 |  |  |  |  |  |  |  |  |  |
| Tetrakis(trimethylsiloxy)silane | 0.3709 | -0.0989 | -0.4768 | -0.7453 |  |  |  |  |  |  |
| Tetramethylorthosilicate | -0.0446 | -0.4203 | -0.7066 |  |  |  |  |  |  |  |
| Toluene | -0.0639 | -0.3955 |  |  |  |  |  |  |  |  |
| Trans Stilbene |  |  | 2.2431 | 1.7274 | 1.3383 | 0.9964 | 0.6592 | 0.3666 | 0.1088 | -0.1127 |
| Tri-n-Butyrin |  |  |  |  |  | 1.2191 | 0.8134 | 0.4624 | 0.1582 | -0.1280 |
| Tribenzylamine |  |  |  |  |  | 1.9349 | 1.5092 | 1.1292 | 0.7986 | 0.5007 |
| Triisopropanolamine |  |  | 2.2786 | 1.7314 | 1.2954 | 0.9685 | 0.6158 | 0.3092 | 0.0346 | -0.1746 |
| Tris(trimethylsiloxy)silane | -0.0860 | -0.5070 | -0.8237 |  |  |  |  |  |  |  |
| Triphenylamine |  |  |  |  |  |  |  | 0.7443 | 0.4550 | 0.1867 |
| Triphenylene |  |  |  |  |  |  |  | 1.6780 | 1.3878 | 1.0122 |
| Triphenylmethane |  |  |  | 2.2831 | 1.8276 | 1.4548 | 1.0925 | 0.7488 | 0.4561 | 0.1829 |
| Valerophenone |  |  |  |  |  | 0.2621 | -0.0109 | -0.2454 | -0.4492 | -0.6764 |
| Vanillin |  |  |  |  | 1.2068 | 0.8820 | 0.5671 | 0.2879 | 0.0345 | -0.1684 |
| Vinyltrimethoxysilane | -0.0349 | -0.3946 | -0.6721 |  |  |  |  |  |  |  |

Table S-8

Retention factor database for Rtx-440 (60-300 °C)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | log60 | log80 | log100 | log120 | log140 | log160 | log180 | log200 | log220 | log240 | log260 | log280 | log300 |
| 1-Acetonaphthone |  |  |  | 1.7282 | 1.3208 | 0.9629 | 0.6697 | 0.4056 | 0.1759 | -0.0258 | -0.2250 | -0.3840 | -0.5440 |
| 1-Bromododecane |  |  |  |  |  | 0.8159 | 0.5146 | 0.2498 | 0.0123 | -0.1939 |  |  |  |
| 1-Bromonaphthalene |  |  |  |  |  | 0.8142 | 0.4993 | 0.2634 | 0.0498 | -0.1361 |  |  |  |
| 1-Chloronaphthalene |  |  |  |  |  | 0.5659 | 0.3143 | 0.0911 | -0.1121 | -0.2882 |  |  |  |
| 1-Hydroxyanthraquinone |  |  |  |  |  |  |  | 1.2241 | 0.9216 | 0.6829 | 0.4462 | 0.2430 | 0.0539 |
| 1-Methylnaphthalene |  |  | 1.3545 | 1.0023 | 0.6896 |  |  |  |  |  |  |  |  |
| 1-Naphthol |  |  |  |  | 1.1264 | 0.8172 | 0.5344 | 0.2837 | 0.0586 | -0.1314 |  |  |  |
| 1-Nitronaphthalene |  |  |  |  |  | 1.0159 | 0.7240 | 0.4662 | 0.2341 | 0.0352 |  |  |  |
| 1-Nitropropane | 0.2808 | -0.0361 |  |  |  |  |  |  |  |  |  |  |  |
| 1-Nitropyrene |  |  |  |  |  |  |  | 1.9657 | 1.6300 | 1.3219 | 1.0508 | 0.7996 | 0.5778 |
| 1-Phenylethanol | 1.4284 | 1.0134 | 0.6560 | 0.3458 | 0.0714 |  |  |  |  |  |  |  |  |
| 1-Phenyl-2-propanol |  | 1.2818 | 0.9078 |  | 0.2644 |  |  |  |  |  |  |  |  |
| 1,12-dodecanediol |  |  |  |  |  | 1.2607 | 0.9144 | 0.6078 | 0.3363 | 0.1068 | -0.1180 | -0.3180 | -0.4900 |
| 1,2-Dichlorobenzene | 1.2763 | 0.8984 | 0.5706 | 0.2819 | 0.0056 | -0.1831 | -0.3743 | -0.5488 | -0.7253 | -0.8365 |  |  |  |
| 1,2-Dimethylbenzene | 0.7858 | 0.4435 | 0.1438 | -0.1233 | -0.3642 | -0.5215 | -0.6971 | -0.8517 |  |  |  |  |  |
| 1,2,4,5-Tetrachlorobenzene | |  | 1.4181 | 1.0599 | 0.7357 |  | 0.1951 | -0.0186 | -0.2312 | -0.3917 | -0.5680 | -0.7040 | -0.8570 |
| 1,2,4-Trichlorobenzene |  | 1.3571 | 0.9888 | 0.6642 | 0.3465 |  |  |  |  |  |  |  |  |
| 1,2,5,6-Dibenzoanthracene | |  |  |  |  |  |  |  |  |  | 1.8503 |  |  |
| 1,3-Dibromobenzene |  | 1.3680 | 1.0036 | 0.6857 | 0.3996 |  |  |  |  |  |  |  |  |
| 1,3-Dichlorobenzene | 1.1790 | 0.8248 | 0.5017 | 0.2161 | -0.0469 |  |  |  |  |  |  |  |  |
| 1,3-Dihydroxybenzene |  |  | 1.3451 | 0.9622 | 0.6174 |  |  |  |  |  | -0.7120 | -0.8580 | -0.9970 |
| 1,3-Dimethylbenzene | 0.7004 | 0.3617 | 0.0652 | 0.2002 | -0.4380 | -0.5865 | -0.7546 | -0.9097 | -1.0860 |  |  |  |  |
| 1,3-Dinitrobenzene |  |  |  |  |  | 0.7351 | 0.4563 | 0.2099 | 0.0079 | -0.1988 | -0.3810 | -0.5350 | -0.6950 |
| 1,3,5-Triethylbenzene |  |  |  |  |  | 0.1207 | 0.1180 | 0.3302 | -0.5319 | -0.6865 |  |  |  |
| 1,4-Dimethylbenzene | 0.6942 | 0.3560 | 0.0594 | 0.2048 | -0.4409 | -0.5835 | -0.7516 | -0.9097 |  |  |  |  |  |
| 1,3-bis(trimethylsiloxy)-1,3-dimethylsilane | 0.9704 | 0.5517 | 0.2016 | -0.1337 | -0.4271 |  |  |  |  |  |  |  |  |
| 1,5-Divinyl-1,1,3,3,5,5-hexamethyltrisiloxane | 1.1736 | 0.7509 | 0.3853 | 0.0564 | -0.2365 |  |  |  |  |  |  |  |  |
| 2-(1-naphthyl)ethanol |  |  |  |  |  | 1.1404 | 0.8332 | 0.5607 | 0.3167 | 0.1047 | -0.0980 | -0.2750 | -0.4350 |
| 2-Acetonaphthone |  |  |  | 1.8092 | 1.3960 | 1.0368 | 0.7407 | 0.4762 | 0.2385 | 0.0325 | -0.1730 | -0.3460 | -0.5100 |
| 2-Chloroacetamide | 0.8388 | 0.4739 | 0.1940 |  |  |  |  |  |  |  |  |  |  |
| 2-Chloroaniline |  | 1.2423 | 0.8787 | 0.5597 | 0.2596 |  |  |  |  |  |  |  |  |
| 2-Chlorophenol | 1.1402 | 0.7669 | 0.4463 | 0.1626 | -0.0885 |  |  |  |  |  | -1.0720 | -1.2120 | -1.3390 |
| 2-Ethoxyethanol | 0.1179 | -0.1856 | -0.4694 |  |  |  |  |  |  |  |  |  |  |
| 2-Heptanone | 0.7391 | 0.3812 | 0.0697 | -0.1991 | -0.4428 |  |  |  |  |  |  |  |  |
| 2-Hexanone | 0.3807 | 0.0526 | -0.2391 | -0.4922 | -0.7324 |  |  |  |  |  |  |  |  |
| 2-Methoxycinnamaldehyde | |  |  | 1.6241 | 1.2121 | 0.8555 | 0.5648 | 0.3025 | 0.0594 |  | -0.3390 | -0.5220 | -0.6660 |
| 2-Methoxyethanol | -0.1503 | -0.4553 |  |  |  |  |  |  |  |  |  |  |  |
| 2-Methoxynaphthalene |  |  |  |  |  | 0.7019 | 0.4305 | 0.2232 | 0.0158 | -0.2137 |  | -0.5730 | -0.7360 |
| 2-Methyl-2-butanol | -0.167 |  |  |  |  |  |  |  |  |  |  |  |  |
| 2-Methylaniline |  |  |  |  |  | -0.0876 | -0.3074 | -0.4881 | -0.6689 | -0.7967 |  |  |  |
| 2-Methylbenzothiazole |  |  |  |  |  |  |  | -0.0598 | -0.2634 | -0.4285 | -0.6037 | -0.7176 | -0.8362 |
| 2-Methylbutanol | 0.2043 | -0.1200 | -0.4081 |  |  |  |  |  |  |  |  |  |  |
| 2-Methylnaphthalene |  |  |  |  |  | 0.3886 | 0.1472 | -0.0671 | -0.2655 | -0.4271 |  |  |  |
| 2-Methylphenol | 1.3937 | 0.9919 | 0.6332 | 0.3180 | 0.0056 | -0.1966 | -0.4040 | -0.5738 | -0.7710 |  |  |  |  |
| 2-Methylpropanol | -0.2253 |  |  |  |  |  |  |  |  |  |  |  |  |
| 2-Naphthol |  |  |  |  |  | 0.8425 | 0.5589 | 0.3074 | 0.0784 | -0.1136 |  |  |  |
| 2-Nitroaniline |  |  |  |  |  | 0.6162 | 0.3560 | 0.1250 | -0.0868 | -0.2629 |  |  |  |
| 2-Nitrophenol |  | 1.2327 | 0.8985 | 0.5811 | 0.2956 | 0.0407 | -0.1674 | -0.3587 | -0.5204 | -0.6146 |  |  |  |
| 2-Nitropropane | 0.1413 |  |  |  |  |  |  |  |  |  |  |  |  |
| 2-Nitrotoluene |  |  |  |  |  | 0.1310 | 0.1369 | 0.3245 | 0.5171 | 0.6616 |  |  |  |
| 2-Nonanone |  | 1.0749 | 0.7004 | 0.3731 | 0.0802 |  |  |  |  |  |  |  |  |
| 2-Octanone | 1.1075 | 0.7142 | 0.3727 | 0.0779 | -0.1856 |  |  |  |  |  |  |  |  |
| 2-Pentanone | 0.0004 | -0.3084 |  |  |  |  |  |  |  |  |  |  |  |
| 2-Phenylacetamide |  |  |  |  | 0.9795 | 0.6198 | 0.3145 | 0.0876 | -0.1221 | -0.3079 | -0.4569 |  |  |
| 2-Phenylethanol |  |  |  |  |  | -0.0252 | -0.2388 | -0.4319 | -0.6093 | -0.7439 |  |  |  |
| 2-Undecanone |  |  |  | 0.9049 | 0.5659 | 0.2649 | 0.0091 | -0.2172 | -0.4301 | -0.5934 |  |  |  |
| 2,3-Dimethylphenol |  | 1.3845 | 0.9873 | 0.6431 | 0.3390 |  |  |  |  |  |  |  |  |
| 2,4-Dimethylaniline |  | 1.2886 | 0.9076 | 0.6118 | 0.3625 |  |  |  |  |  |  |  |  |
| 2,4-Dinitroaniline |  |  |  |  |  | 1.6823 | 1.3373 | 1.0235 | 0.8246 | 0.5044 |  |  |  |
| 2,6-Dichloro-4-nitroaniline | |  |  |  |  | 1.2470 | 0.9328 | 0.6567 | 0.4018 | 0.1832 | 0.0150 |  |  |
| 2,6-Dimethylphenol |  | 1.1694 | 0.8015 | 0.4771 | 0.2596 |  |  |  |  |  |  |  |  |
| 2,2,4,4,6,6-Hexamethylcyclotrisilazane | 1.3653 | 0.9425 | 0.5706 | 0.2494 | -0.0458 |  |  |  |  |  |  |  |  |
| 2,4,6,8-tetramethyl-2,,4,6,8-tetravinylcyclosiloxane | | | 1.1141 | 0.7261 | 0.3770 |  |  |  |  |  |  |  |  |
| 3-Aminopropyltriethoxysilane | |  |  |  |  | 0.1474 | -0.1138 | -0.3387 | -0.5540 | -0.7253 | -0.9170 | -1.0620 | -1.2460 |
| 3-Methylaniline |  |  |  |  |  | -0.0889 | -0.2963 | -0.4856 | -0.6665 | -0.7984 |  |  |  |
| 3-Methylbutanol | 0.2137 | -0.1154 | -0.4110 |  |  |  |  |  |  |  |  |  |  |
| 3-Methylphenol | 1.5310 | 1.0802 | 0.7323 | 0.4044 | 0.1509 | -0.1566 | -0.3678 | -0.5507 | -0.7352 |  |  |  |  |
| 3-Nitroaniline |  |  |  |  |  | 0.7827 | 0.5035 | 0.2568 | 0.0376 | -0.1537 |  |  |  |
| 3-Nitrotoluene |  |  |  |  |  | 0.2189 | 0.0395 | -0.2458 | -0.4387 |  |  |  |  |
| 3-Phenylpropan-1-ol |  |  | 1.1365 | 0.7823 | 0.4702 |  |  |  |  |  |  |  |  |
| 3,3'-Dichlorobenzidine |  |  |  |  |  |  |  | 1.7987 | 1.4593 |  | 0.8731 | 0.6240 | 0.3976 |
| 3,4-Dichloroanilne |  |  |  |  |  | 0.6617 | 0.3955 | 0.1623 | -0.0561 | -0.2408 |  |  |  |
| 3,5-Dimethylphenol |  | 1.3562 | 0.9539 | 0.6067 | 0.3010 | 0.0551 | -0.1697 | -0.3678 | -0.5569 | -0.7088 |  |  |  |
| 4-acetylbiphenyl |  |  |  |  |  | 1.4408 | 1.1040 | 0.8052 | 0.5373 | 0.2990 |  |  |  |
| 4-Bromoacetanilide |  |  |  |  |  |  | 0.8537 | 0.5658 | 0.3210 | 0.1140 |  |  |  |
| 4-Chloro-2-nitroaniline |  |  |  |  |  | 0.9904 | 0.6997 | 0.4302 | 0.2053 | 0.0068 |  |  |  |
| 4-Chloroaniline |  |  |  |  |  | 0.1874 | -0.0380 | -0.2432 | -0.4315 | -0.5812 |  |  |  |
| 4-Chlorophenol |  | 1.4344 | 1.0248 | 0.6710 | 0.3629 | 0.1141 | -0.1200 | -0.3141 | -0.5161 | -0.6473 |  |  |  |
| 4-Cyanophenol |  |  |  | 1.2940 | 0.8991 | 0.5727 | 0.2925 | 0.0565 | -0.1711 | -0.3449 |  |  |  |
| 4-Dimethylaminoazobenzene | |  |  |  |  |  |  | 1.2093 | 0.9145 | 0.6446 | 0.4006 | 0.1880 | -0.0094 |
| 4-Fluoroaniline | 1.2405 | 0.8620 | 0.5209 | 0.2190 | -0.0528 | -0.2675 | -0.4699 | -0.6342 | -0.8241 | -0.9028 | -1.0830 | -1.2310 |  |
| 4-Hydroxybenzaldehyde |  |  |  |  | 0.7955 | 0.4787 | 0.2126 | -0.0177 | -0.2332 | -0.4078 |  |  |  |
| 4-Hydroxybezyl alcohol |  |  |  | 1.1457 | 0.7716 | 0.4606 | 0.1947 | -0.0340 | -0.2261 | -0.4194 |  |  |  |
| 4-Methoxy-2-nitroaniline |  |  |  |  |  | 1.0592 | 0.7599 | 0.4820 | 0.2479 | 0.0401 |  |  |  |
| 4-Methoxybenzyl alcohol |  |  | 1.3591 | 0.9812 | 0.6356 | 0.3485 | 0.0966 | -0.1202 | -0.3436 | -0.5037 | -0.6740 | -0.8160 |  |
| 4-Methylphenol | 1.5068 | 1.0578 | 0.7256 | 0.3992 | 0.1509 | -0.1601 | -0.3633 | -0.5526 | -0.7367 | -0.8419 |  |  |  |
| 4-Nitroaniline |  |  |  |  |  | 1.0243 | 0.7289 | 0.4646 | 0.2335 | 0.0201 |  |  |  |
| 4-Nitrobenzyl alcohol |  |  |  | 1.6319 | 1.2232 | 0.8713 | 0.5812 | 0.3261 | 0.0851 | -0.1088 | -0.2920 | -0.4690 | -0.6540 |
| 4-Nitrotoluene |  |  |  |  |  | 0.2192 | -0.0085 | -0.2079 | -0.4026 | -0.5418 |  |  |  |
| 4,4'-Dibromobiphenyl |  |  |  |  |  |  |  | 1.0892 | 0.8105 | 0.5590 | 0.3288 | 0.1300 | -0.0538 |
| 4,4'-Methylenedianiline |  |  |  |  |  |  | 1.6198 | 1.2887 | 0.9802 | 0.7222 | 0.4686 |  |  |
| 8-Hydroxyquinoline |  |  |  |  |  |  |  | 0.0475 | -0.1468 | -0.3168 | -0.4958 | -0.6273 | -0.7800 |
| Acenaphthene |  |  |  |  |  |  |  |  |  |  | -0.3210 | -0.4750 | -0.6110 |
| Acenaphthylene |  |  |  |  |  | 0.7130 | 0.4527 | 0.2178 | 0.0066 |  | -0.3480 | -0.5070 | -0.6500 |
| Acetamide | 0.5495 | 0.1650 | 0.1350 |  |  |  |  |  |  |  |  |  |  |
| Acetoacetanilide | 1.3692 | 1.0280 | 0.7001 | 0.4334 | 0.2036 |  |  |  |  |  |  |  |  |
| Acetophenone | 1.4412 | 1.0747 | 0.7233 | 0.4116 | 0.0985 | -0.1187 | -0.3243 | -0.5012 | -0.6943 | -0.8136 |  |  |  |
| alpha-Isomethyl ionone |  |  | 1.7988 | 1.3909 | 1.0024 | 0.6731 | 0.3946 | 0.1515 | -0.0811 | -0.2700 | -0.4500 | -0.6230 | -0.7790 |
| alpha-Pinene |  |  | 0.2197 | -0.0589 | -0.2917 | -0.4684 | -0.6612 | -0.8011 | -0.9521 | -1.0419 | -1.2560 |  |  |
| Amyl cinnamal |  |  |  |  | 1.4289 | 1.0464 | 0.7343 | 0.4580 | 0.1964 | -0.0163 | -0.2150 | -0.4010 | -0.5610 |
| Androsterone |  |  |  |  |  |  |  |  |  | 1.2487 | 0.9620 | 0.7110 | 0.4840 |
| Aniline | 1.1437 | 0.7633 | 0.4340 | 0.1464 | -0.1119 | -0.3090 | -0.4985 | -0.6670 | -0.8418 | -0.9425 |  |  |  |
| Anisole |  |  |  |  |  | -0.4758 | -0.6488 | -0.8141 | -0.9937 |  |  |  |  |
| Anthracene |  |  |  |  |  | 1.3705 | 1.0558 | 0.7765 | 0.5246 | 0.3018 | 0.0960 | -0.0910 | -0.2570 |
| Anthraquinone |  |  |  |  |  |  |  | 1.0574 | 0.7652 | 0.5401 | 0.3136 | 0.1172 | -0.0642 |
| Azulene |  |  |  |  |  |  |  | -0.0222 | -0.2118 | -0.3814 | -0.5571 | -0.6657 | -0.8189 |
| Benz[a]anthracene |  |  |  |  |  |  |  | 1.7485 | 1.4115 | 1.1321 | 0.8714 | 0.6331 | 0.4209 |
| Benzaldehyde | 1.0878 | 0.7195 | 0.3952 | 0.1113 | -0.1428 | -0.3350 | -0.5189 | -0.6870 | -0.8644 | -0.9472 |  |  |  |
| Benzamide |  |  | 1.4811 | 1.0893 | 0.7487 | 0.4585 | 0.2089 | -0.0216 | -0.2239 | -0.3906 |  |  |  |
| Benzene | -0.1068 | -0.3835 |  |  |  |  |  |  |  |  |  |  |  |
| Benzenesulfonamide |  |  |  |  |  | 0.9220 | 0.6276 | 0.3690 | 0.1324 | -0.0699 | -0.2540 | -0.4230 | -0.5750 |
| Benzidine |  |  |  |  |  |  |  | 1.2947 | 0.9900 | 0.7174 | 0.4706 | 0.2538 | -0.0555 |
| Benzodioxane |  | 1.3739 | 1.0029 | 0.6745 | 0.3465 |  |  |  |  |  |  |  |  |
| Benzo[a]pyrene |  |  |  |  |  |  |  |  | 1.9257 | 1.5974 | 1.3110 | 1.0424 | 0.8074 |
| Benzo[e]pyrene |  |  |  |  |  |  |  |  | 1.9058 | 1.5800 | 1.2940 | 1.0252 | 0.7898 |
| Benzo[ghi]perylene |  |  |  |  |  |  |  |  |  | 2.1504 | 1.8640 |  |  |
| Benzonitrile | 1.1256 | 0.7528 | 0.4288 | 0.1467 | -0.1051 |  |  |  |  |  |  |  |  |
| Benzophenone |  |  |  |  |  | 1.0439 | 0.7445 | 0.4741 | 0.2326 | 0.0236 |  |  |  |
| Benzothiazole |  |  |  |  |  |  |  | -0.1650 | -0.3522 | -0.5127 | -0.6838 | -0.8069 | -0.9431 |
| Benzyl 2-ethylhexyl phthalate | |  |  |  |  |  |  |  | 1.4621 | 1.1166 |  |  | 0.4393 |
| Benzyl alcohol | 1.4212 | 0.9875 | 0.6421 | 0.3244 | 0.0696 | -0.1966 | -0.4001 | -0.5679 | -0.7588 | -0.8782 |  |  |  |
| Benzyl cinnamate |  |  |  |  |  |  | 1.5655 | 1.2187 | 0.9115 | 0.6377 | 0.3860 | 0.1580 | -0.0450 |
| Benzyl salicylate |  |  |  |  |  | 1.5052 | 1.1649 | 0.8539 | 0.5783 | 0.3388 | 0.1130 | -0.0890 | -0.2650 |
| beta-Pinene |  |  |  |  |  | -0.3504 | -0.5455 | -0.6944 | -0.9521 | -1.0419 |  |  |  |
| Bis(trimethylsiloxy)methylsilane | 0.4268 | 0.0632 | -0.1882 | -0.5370 |  |  |  |  |  |  |  |  |  |
| Borneol |  | 1.3156 | 0.9432 | 0.6166 | 0.3308 |  | -0.1264 | -0.3209 | -0.5109 | -0.6386 | -0.7950 | -0.9410 | #NULL! |
| Bromobenzene | 0.9201 | 0.5724 | 0.2696 | 0.0065 | -0.2272 |  |  |  |  |  |  |  |  |
| Butan-1-ol | -0.1022 | -0.4114 |  |  |  |  |  |  |  |  |  |  |  |
| n-Butylbenzene | 1.3424 | 0.9636 | 0.6180 | 0.3128 | 0.0365 |  |  |  |  |  |  |  |  |
| Butyl acetate | 0.4509 | 0.1085 | -0.1943 | -0.4577 | -0.7324 |  |  |  |  |  |  |  |  |
| Butyl benzoate |  |  | 1.5050 | 1.1239 | 0.7789 |  |  |  |  |  |  |  |  |
| Butyl benzyl phthalate |  |  |  |  |  |  |  | 1.5749 | 1.2285 | 0.9215 | 0.6500 | 0.3980 | 0.1720 |
| Butyl cyclohexyl phthalate |  |  |  |  |  |  |  | 1.3648 | 1.0462 | 0.7538 | 0.4930 | 0.2530 |  |
| Butyl decyl phthalate |  |  |  |  |  |  | 1.2673 | 0.9344 | 0.6349 | 0.3726 | 0.1349 | -0.0827 | -0.2724 |
| Butyl 2-ethylhexyl phthalate | |  |  |  |  |  |  |  | 1.4588 | 1.1164 |  |  |  |
| Butyl octyl phthalate |  |  |  |  |  |  | 1.2677 | 0.9325 | 0.6599 | 0.3719 | 0.1336 | -0.0813 | -0.2724 |
| Butyl oleate |  |  |  |  |  |  |  | 1.5461 | 1.1945 | 0.8731 | 0.5810 | 0.3150 | 0.0860 |
| Butyl stearate |  |  |  |  |  |  |  |  | 1.2633 | 0.9023 | 0.6040 | 0.3250 | 0.1000 |
| Camphor |  | 1.2780 | 0.9143 | 0.5891 | 0.2998 | 0.0500 | -0.1661 | -0.3493 | -0.5326 | -0.6716 | -0.8230 | -0.9590 |  |
| Carbazole |  |  |  |  |  | 1.4804 | 1.1498 | 0.8539 | 0.5911 | 0.3571 | 0.1470 | -0.0460 | -0.2190 |
| Carbon tetrachloride | -0.1188 | -0.3958 |  |  |  |  |  |  |  |  |  |  |  |
| Carvone |  |  | 1.2007 | 0.8472 | 0.5165 | 0.2438 | 0.0072 | -0.2026 | -0.4038 | -0.5682 | -0.7170 | -0.8590 | -1.0020 |
| Chlorobenzene | 0.6107 | 0.2873 | 0.0041 | -0.2468 | -0.4740 |  |  |  |  |  |  |  |  |
| Chloroform | -0.2758 |  |  |  |  |  |  |  |  |  |  |  |  |
| Cholestane |  |  |  |  |  |  |  |  |  | 1.5122 | 1.2000 | 0.9220 | 0.6720 |
| Cholesteryl acetate |  |  |  |  |  |  |  |  |  |  |  |  | 1.0260 |
| Chrysene |  |  | 0.8847 | 1.0432 | 0.7238 | 0.3937 | 0.1379 | -0.0834 | 1.4410 | 1.1482 | 0.8910 | 0.6410 | 0.4240 |
| Cinnamyl alcohol |  |  |  | 0.5436 | 0.2284 | -0.0205 | -0.2553 | -0.4449 | -0.2946 | -0.4631 |  |  |  |
| Citronellal |  |  |  |  |  | 0.7030 | 0.4360 | 0.2018 | -0.6372 | -0.7783 | -0.9450 | -1.1120 |  |
| Coumarin | 0.8137 | 0.4549 | 0.1429 |  |  |  |  |  | -0.0122 | -0.1663 | -0.3720 | -0.5250 | -0.6720 |
| Cycloheptanone | 0.8026 | 0.4590 | 0.1588 | -0.1286 | -0.3773 |  |  |  |  |  |  |  |  |
| Cyclohexanol |  | 1.0008 | 0.6465 | -0.1037 | -0.3428 |  |  |  |  |  |  |  |  |
| Cyclohexanone |  |  |  | 0.3373 | 0.0413 | -0.1677 | -0.3675 |  |  |  |  |  |  |
| Cyclohexanone oxime |  |  |  |  |  |  |  |  | -0.7295 | -0.8419 |  |  |  |
| Decaethylcyclopentasiloxane | 1.2196 | 0.7791 | 0.3984 |  |  |  |  |  |  |  |  |  |  |
| Decamethylcyclopentasiloxane | |  | 1.1930 | 0.0559 |  |  |  |  |  |  |  |  |  |
| Decamethyltetrasiloxane | 1.0802 | 0.6891 | 0.3481 | 0.8159 | 0.4845 | 0.2131 | -0.0394 | -0.2620 |  |  |  |  |  |
| Decan-1-ol |  |  |  | 0.0495 | -0.2208 | -0.3762 | -0.5618 | -0.7273 | -0.4702 | -0.6324 |  |  |  |
| Decane |  |  |  |  |  |  | 1.3716 | 1.0264 | -0.9177 |  |  |  |  |
| Di-(2-Methoxyethyl) phthalate | |  |  |  |  |  |  |  | 0.7207 | 0.4472 | 0.2010 | -0.0220 | -0.2170 |
| Di-2-ethylhexyl phthalate |  |  |  |  |  |  | 1.2744 | 0.9377 | 1.4636 | 1.1170 | 0.8450 | 0.5300 | 0.2820 |
| Di-n-Butyl phthalate |  |  |  |  |  |  | 0.5154 | 0.2409 | 0.6401 | 0.3744 | 0.1370 | -0.0810 | -0.2770 |
| Di-n-Butyl succinate |  |  |  |  |  |  |  |  | -0.0156 | -0.2235 | -0.4340 | -0.6100 | -0.7800 |
| Di-n-Octyl phthalate |  |  |  |  |  |  | 1.5754 | 1.2060 | 1.7622 | 1.3877 | 1.0570 | 0.7580 | 0.4950 |
| Di(2-Ethoxyethyl) phthalate | |  |  |  |  |  |  |  | 0.8840 | 0.5906 | 0.3290 | 0.0960 | -0.1160 |
| Di(2-n-butoxyethyl) phthalate | |  |  |  |  | 0.8337 | 0.5596 | 0.3153 | 1.4044 | 1.0635 | 0.7620 | 0.4880 | 0.2460 |
| Dibenzofuran |  |  |  |  | 1.4521 | 1.0736 | 0.7636 | 0.4889 | 0.0938 | -0.0974 |  |  |  |
| Dibenzyl ether |  |  |  |  |  | 1.2233 | 0.9016 | 0.6171 | 0.2423 | 0.0254 | -0.1690 | -0.3670 |  |
| Dibenzylamine |  |  |  |  |  |  |  |  | 0.3618 | 0.1366 |  |  |  |
| Dicyclohexyl phthalate |  |  |  |  |  | 0.5995 | 0.3100 | 0.0586 | 1.4431 | 1.1264 | 0.8420 | 0.5820 | 0.3450 |
| Dicyclohexylamine | 0.2313 | -0.1178 | -0.3174 |  |  |  |  | 1.4816 | -0.1386 | -0.3159 | -0.5049 |  |  |
| Dicylcohexyl adipate |  |  |  | -0.6811 | -0.9507 |  |  |  | 1.1443 | 0.8428 |  |  |  |
| Diethoxydimethylsilane |  |  |  |  |  |  | 0.1778 | -0.0690 |  |  |  |  |  |
| Diethyl adipate |  |  |  |  |  |  | -0.0398 | -0.2638 | -0.3001 | -0.4869 | -0.6780 | -0.8450 | -0.9730 |
| Diethyl diethylmalonate |  |  |  |  | 1.3098 | 0.9332 | 0.6252 | 0.3511 | -0.4763 | -0.6532 | -0.8180 | -0.9320 |  |
| Diethyl phthalate |  |  |  |  |  |  | 0.9454 | 0.6272 | 0.0928 | -0.1133 | -0.3120 | -0.4830 | -0.6490 |
| Diethyl sebecate |  |  |  |  |  |  |  |  | 0.3414 | 0.0955 | -0.1310 | -0.3370 | -0.5180 |
| Dihydrocholesterol |  |  |  |  |  | 1.4494 | 1.0897 | 0.7709 |  |  |  |  |  |
| Diisobutyl phthalate | 0.1245 | -0.1818 |  |  |  |  | 0.3864 | 0.1388 | 0.4863 | 0.2360 | 0.0140 | -0.1930 | -0.3780 |
| Dimethyl phthalate |  |  |  |  |  |  |  |  | -0.1035 | -0.2852 | -0.4730 | -0.6450 | -0.7810 |
| Dioxane |  |  |  | 1.2489 | 0.8842 | 0.5742 | 0.3104 | 0.0779 |  |  |  |  |  |
| Diphenyl ether |  | 1.6185 | 1.1391 |  | 1.4454 | 1.0402 | 0.7344 | 0.4638 | -0.1348 | -0.3185 |  |  |  |
| Diphenylamine |  | 1.3570 | 0.8979 | 0.7415 | 0.3822 | 0.0999 | -0.1635 | -0.3944 | 0.2208 | 0.0112 |  |  |  |
| Dodecamethylcyclohexasiloxane | | 1.3379 | 0.9343 | 0.5136 | 0.1665 |  |  |  | -0.6125 | -0.7789 |  |  |  |
| Dodecamethylpentasiloxane | |  |  | 0.5822 | 0.2695 | 0.0132 | -0.2235 | -0.4333 |  |  |  |  |  |
| Dodecane | -0.3425 |  |  |  |  |  |  |  | -0.6335 | -0.7789 |  |  |  |
| Dodecanol |  | 1.3273 | 0.9418 |  |  |  |  |  |  |  |  |  |  |
| Ethyl acetate | 0.5823 | 0.2309 | -0.0781 | 0.6065 | 0.3083 |  |  |  |  |  |  |  |  |
| Ethyl benzoate |  |  |  | -0.3483 | -0.5931 |  |  |  |  |  |  |  |  |
| Ethyl 2-methylbutyrate | 0.0935 |  |  |  |  |  |  | 1.1447 |  |  |  |  |  |
| Ethyl oleate | 0.6543 | 0.3199 | 0.0271 |  |  |  |  |  | 0.9096 | 0.6120 | 0.3420 | 0.1030 | -0.1150 |
| Ethyl propionate |  |  | 1.5226 | -0.2323 | -0.4678 |  |  |  |  |  |  |  |  |
| Ethylbenzene |  |  |  | 1.1350 | 0.7686 | 0.4637 | 0.1983 | -0.0287 |  |  |  |  |  |
| Eugenol |  |  |  |  |  |  | 1.4978 | 1.1850 | -0.2497 | -0.4294 | -0.6010 | -0.7530 | -0.9160 |
| Fluoranthene |  |  | 1.2502 |  |  | 0.9954 | 0.6825 | 0.4277 | 0.9037 | 0.6517 | 0.4280 | 0.2190 | 0.0360 |
| Fluorene |  |  | 1.1958 | 0.8794 | 0.5315 | 0.2478 |  | -0.2166 | 0.1989 | -0.0016 | -0.1880 | -0.3570 | -0.5100 |
| Geranial |  |  | 1.7700 | 0.8211 | 0.4752 | 0.1971 | -0.0544 | -0.2659 | -0.4301 | -0.5934 |  |  |  |
| Geraniol | 0.8036 | 0.4404 | 0.1238 | 1.3333 | 0.9365 | 0.6109 | 0.3142 | 0.0579 | -0.4811 | -0.6470 | -0.8100 | -0.9560 |  |
| Glycidoxypropyltrimethoxysilane | -0.0544 | -0.3512 | -0.6138 | -0.1536 | -0.4066 |  |  |  | -0.1859 | -0.3855 | -0.5940 | -0.7440 | -0.9180 |
| heptanol |  |  |  |  |  | 1.1908 | 0.8855 | 0.6159 |  |  |  |  |  |
| Hexachlorobenzene |  |  | 1.5129 |  |  | 0.8519 | 0.5380 | 0.2693 | 0.3718 | 0.1575 | -0.0430 | -0.2200 | -0.3860 |
| Hexadecane | 0.3805 | 0.0221 | -0.2147 | 1.1062 | 0.7355 |  |  |  | 0.0071 | -0.2081 |  |  |  |
| Hexaethylcyclotrisiloxane | 0.0496 | -0.2780 | -0.4156 | -0.5639 |  |  |  |  |  |  |  |  |  |
| Hexamethylcyclotrisiloxane | 0.9174 | 0.5511 | 0.2419 | -0.7943 | -1.0364 |  |  |  |  |  |  |  |  |
| Hexamethyldisilane | 0.3040 | -0.0358 | -0.2443 | -0.0560 | -0.3020 |  |  |  |  |  |  |  |  |
| Hexamethyldisilathiane | -0.1215 | -0.4806 |  | -0.5831 | -0.8301 |  |  |  |  |  |  |  |  |
| Hexanal | 0.6949 | 0.3281 | 0.0146 |  |  |  |  |  |  |  |  |  |  |
| Hexane |  |  | 1.3286 | -0.2643 | -0.5098 |  |  |  |  |  |  |  |  |
| Hexanol | 1.2818 | 0.9090 | 0.5839 | 0.9440 | 0.5864 | 0.2965 | 0.0383 | -0.1802 |  |  |  |  |  |
| Hydroxycitronellal |  |  |  | 0.3007 | 0.0470 | -0.1462 | -0.3402 | -0.5139 | -0.3985 | -0.5612 |  |  |  |
| Iodobenzene |  |  |  |  |  | 0.3427 | 0.0657 | -0.1731 | -0.6891 | -0.8034 |  |  |  |
| Isocyanatopropyltriethoxysilane | |  | 0.5148 | 1.5672 | 1.1594 |  |  |  | -0.4032 | -0.5822 | -0.7890 | -0.9300 | -1.0910 |
| Lilial | 1.5168 | 1.0824 | 0.7079 | 0.2167 | -0.0547 | -0.2563 | -0.4615 | -0.6374 |  |  | -0.3860 | -0.5580 |  |
| Limonene |  |  | 1.6730 | 0.3823 | 0.0931 | -0.1331 | -0.3557 | -0.5475 | -0.8034 | -0.9126 |  |  |  |
| Linalool |  |  |  | 1.2405 | 0.8476 | 0.5258 | 0.2314 | -0.0274 | -0.7307 | -0.8605 |  |  |  |
| Methacryloxypropyltrimethoxysilane | 1.5189 | 1.1033 | 0.7429 |  |  |  |  |  | -0.2646 | -0.4616 | -0.6690 | -0.8220 | -0.9920 |
| Methyl abietate |  |  |  |  |  |  |  |  | 1.2207 | 0.9196 | 0.7090 | 0.4640 | 0.2420 |
| Methyl benzoate |  |  | 1.3473 |  |  |  |  |  |  |  |  |  |  |
| Methyl Cyclohexane |  |  | 1.6645 | 0.9536 | 0.6060 |  |  |  |  |  |  |  |  |
| Methyl decanoate | 0.8611 | 0.4854 | 0.1580 | 1.2506 | 0.8591 | 0.5297 | 0.2547 | 0.0104 |  |  |  |  |  |
| Methyl eugenol |  | 1.4795 | 1.0589 | -0.1276 | -0.3857 |  |  |  | -0.2189 | -0.4013 | -0.5840 | -0.7650 | -0.9070 |
| Methyl hexanoate |  | 1.1544 | 0.7653 | 0.6927 | 0.3683 |  | -0.1485 | -0.3557 |  |  |  |  |  |
| Methyl nonanoate |  |  |  | 0.4263 | 0.1252 |  |  |  | -0.5138 | -0.6564 | -0.8560 | -1.0230 |  |
| Methyl octanoate | 0.8396 | 0.4462 | 0.1257 |  |  |  |  |  |  |  |  |  |  |
| Methyl phenyl ether | 0.6452 | 0.2921 | 0.0004 | -0.2006 | -0.4700 |  |  |  |  |  |  |  |  |
| Methylbis(trimethylsiloxy)vinylsilane | 1.1432 | 0.7127 | 0.3455 | -0.3292 | -0.5968 |  |  |  |  |  |  |  |  |
| Methyltriethoxysilane | 0.6813 | 0.3319 | 0.0680 | 0.0060 | -0.2896 |  |  |  |  |  |  |  |  |
| N-Methylaniline |  |  |  |  |  | 1.5171 | 1.1798 | 0.8791 |  |  |  |  |  |
| N,N-Diethyl-4-nitroaniline | |  |  |  |  | 1.4822 | 1.1480 | 0.8412 | 0.6077 | 0.3797 |  |  |  |
| N,N-Diethylcarbanilide |  |  |  |  |  | 1.6074 | 1.2331 | 0.8970 | 0.5845 | 0.3432 | 0.1120 | -0.0870 | -0.2600 |
| N,N-Diethyldodecamide | 1.5852 | 1.1824 | 0.8622 |  |  | 1.2494 | 0.9419 | 0.6597 | 0.5982 | 0.3389 | 0.0850 | -0.1280 | -0.3150 |
| N,N-Dimethyl-4-nitroaniline | |  |  |  | 0.1816 | -0.0407 |  |  |  |  |  |  |  |
| N,N-Dimethylaniline |  | 1.3683 | 1.0003 |  |  |  |  |  |  |  |  |  |  |
| N,N-Diphenyl-4-phenylenediamine | |  | 1.1593 | 0.6800 | 0.3953 | 0.1658 | -0.0529 | -0.2469 | 1.6464 | 1.3212 | 1.1000 | 0.8250 | 0.5790 |
| Naphthalene |  |  |  | 0.7994 | 0.4622 | 0.1889 | -0.0522 | -0.2642 | -0.4294 | -0.5762 |  |  |  |
| Neral |  |  | 1.4678 | 1.2910 | 0.9117 | 0.5933 | 0.3246 | 0.0900 | -0.4714 | -0.5934 |  |  |  |
| Nicotinamide | 1.5046 | 1.1046 | 0.7558 | 1.0994 | 0.7510 | 0.4611 | 0.2102 | -0.0079 | -0.1373 | -0.3069 | -0.4890 | -0.6410 | -0.7750 |
| Nicotine | 1.5310 | 1.1126 | 0.7175 | 0.4494 | 0.1977 |  |  |  | -0.2219 | -0.3415 | -0.5570 | -0.7000 | -0.8180 |
| Nitrobenzene | 0.7079 | 0.3519 | 0.0398 | 0.4066 | 0.1135 |  |  |  |  |  |  |  |  |
| Nonanal |  |  |  | -0.2330 | -0.4824 | -0.6326 | -0.8020 | -0.9692 |  |  |  |  |  |
| Nonane |  |  |  |  |  |  |  |  | -1.1709 |  |  |  |  |
| Nonanol |  |  |  |  |  | 1.2657 | 0.9112 | 0.5983 |  |  |  |  |  |
| Octadecane | 0.9786 | 0.5621 | 0.2137 |  | 1.4078 | 1.0392 | 0.7057 | 0.4122 | 0.3187 | 0.0718 |  |  |  |
| Octaethylcyclotetrasiloxane | 0.5507 | 0.1769 | -0.0980 |  | -0.4037 |  |  |  | 0.1461 | -0.0809 |  |  |  |
| Octamethylcyclotetrasiloxane | 1.4539 | 1.0341 | 0.6547 | -0.4356 | -0.7079 |  |  |  |  |  |  |  |  |
| Octamethyltrisiloxane | 1.1596 | 0.7535 | 0.4030 | 0.3244 |  |  |  |  |  |  |  |  |  |
| Octan-1-ol | 1.1449 | 0.7502 | 0.4082 | 0.0991 | -0.1714 | -0.3686 | -0.5749 | -0.7407 |  |  |  |  |  |
| Octan-2-ol | 0.3345 | 0.0107 | -0.2768 | 0.1124 | -0.1506 |  |  |  | -0.9219 | -1.0071 | -1.2250 | -1.3570 | #NULL! |
| Octanal |  |  |  | -0.5260 |  |  |  |  |  |  |  |  |  |
| Octane |  |  |  |  |  | 1.0855 | 0.7656 |  |  |  |  |  |  |
| Octanophenone |  |  |  |  |  |  |  |  | 0.2284 | 0.0052 | #NULL! | #NULL! | -0.5490 |
| Octyltriethoxysilane | 0.3385 | 0.0031 | -0.2977 |  |  | 1.2836 | 0.9676 | 0.6870 |  |  | -0.6550 | -0.8040 | -0.9970 |
| Pentachlorophenol | 0.0624 | -0.2574 |  |  |  |  |  |  | 0.4366 | 0.2150 |  |  |  |
| Pentan-1-ol | 0.0683 | -0.2492 | -0.5343 |  |  |  |  |  |  |  |  |  |  |
| Perylene | 1.1285 | 0.7506 | 0.4083 |  |  | 1.3465 | 1.0358 | 0.7577 |  |  |  |  | 0.8220 |
| Phenanthrene | 1.4173 | 1.0145 | 0.6535 | 0.1037 |  | -0.3762 | -0.5618 | -0.7273 | 0.5058 | 0.2842 | 0.0800 | -0.1010 | -0.2690 |
| Phenol |  |  | 1.3786 | 0.3391 | 0.0594 | -0.1783 | -0.3825 | -0.5583 | -0.9117 |  |  |  |  |
| Phenylacetate | 0.3737 | 0.0560 | -0.1492 | 1.0199 | 0.6838 | 0.4026 | 0.1609 | -0.0589 | -0.7528 | -0.8531 |  |  |  |
| Phenylcyclohexane |  |  |  | -0.4614 | -0.6908 |  |  |  | -0.2607 | -0.4257 |  | -0.7680 | -0.8740 |
| Phenyltrimethoxysilane |  |  |  |  |  | 0.7491 | 0.4684 | 0.2220 |  |  |  |  |  |
| Phthalimide |  |  |  |  |  | 0.4467 | 0.1952 | -0.0233 | 0.0024 | -0.1869 |  |  |  |
| Phthalonitrile | 0.0648 | -0.2512 | -0.5343 |  |  |  |  |  | -0.2265 | -0.3991 |  |  |  |
| Progesterone |  |  |  | -0.7832 | -0.8531 |  |  |  |  |  |  | 1.0110 | 0.7610 |
| Propyl acetate |  |  |  |  |  |  | 1.5811 | 1.2653 |  |  |  |  |  |
| Pyrene |  |  |  |  |  |  |  |  | 0.9815 | 0.7266 |  |  |  |
| Quinine | 0.7757 | 0.4327 | 0.1330 |  |  | 0.2836 | 0.0563 | -0.1494 | 1.9820 | 1.6183 | 1.3025 | 1.0092 | 0.7518 |
| Quinoline |  |  |  | -0.1315 | -0.3690 |  |  |  | -0.3412 | -0.5446 | -0.6500 | -0.7960 | -0.9120 |
| Styrene |  | 1.3406 | 0.9592 |  |  |  |  | 1.3592 |  |  |  |  |  |
| p-Terphenyl |  |  |  | 0.6260 | 0.3334 | 0.0964 | -0.1339 | -0.3260 | 1.0506 | 0.7723 | 0.5210 | 0.3004 | 0.0978 |
| Terpinen-4-ol | 1.0490 | 0.6351 | 0.2836 |  |  |  |  |  | -0.5167 | -0.6587 | -0.8210 |  |  |
| n-Tetradecane | -0.2424 |  |  | -0.0469 | -0.3239 |  |  |  |  |  |  |  |  |
| Tetraethylorthosilicate | 1.6170 | 1.1373 | 0.7136 |  |  |  |  |  |  |  |  |  |  |
| Tetrahydofuran | 0.3155 | -0.0340 |  | 0.3528 | 0.0262 |  |  |  |  |  |  |  |  |
| Tetrakis(trimethylsiloxy)silane | |  |  | -0.5999 |  |  |  |  |  |  |  |  |  |
| Tetramethylorthosilicate | 0.2942 | 0.0004 | -0.2726 |  |  |  |  |  |  |  |  |  |  |
| Thioacetamide |  |  |  | -0.5059 |  |  |  |  |  |  |  |  |  |
| Toluene |  |  |  |  |  | 1.1995 | 0.8859 | 0.6048 |  |  |  |  |  |
| Trans Stilbene |  |  |  |  |  | 1.4251 | 1.0484 | 0.7151 | 0.3530 | 0.1299 | -0.0750 | -0.2550 | -0.4250 |
| Tri-n-Butyrin |  |  | 1.2171 |  |  |  |  | 1.4817 | 0.4205 | 0.1615 | -0.0760 | -0.2850 | -0.4750 |
| Tribenzylamine | -0.0748 | -0.3743 |  | 0.8374 | 0.5014 |  |  |  | 1.1613 | 0.8682 | 0.5980 | 0.3610 | 0.1460 |
| Triethylamine | 1.0471 | 0.6212 | 0.2639 | 1.3133 | 0.9152 | 0.6423 | 0.3603 | 0.1096 |  |  |  |  |  |
| Triisopropanolamine |  |  |  | -0.0738 | -0.3678 |  |  |  | -0.1241 | -0.3166 | -0.5010 | -0.6570 | -0.8090 |
| Trimethoprin |  |  |  |  |  |  | 1.4128 | 1.0853 |  |  | 1.0230 | 0.7440 | 0.4950 |
| Triphenylamine |  |  |  |  |  |  |  | 1.7576 | 0.7925 |  | 0.2970 | 0.0880 | -0.1080 |
| Triphenylene | 1.4348 | 1.0070 | 0.6354 |  |  | 1.7422 | 1.3739 | 1.0485 | 1.4335 | 1.1426 | 0.8788 | 0.6395 | 0.4274 |
| Triphenylmethane | 0.0165 | -0.2825 | -0.5459 | 0.3116 | 0.0222 | -0.1999 | -0.4169 | -0.6066 | 0.7576 | 0.4977 | 0.2670 | 0.0530 | -0.1460 |
| Undecane |  |  |  |  |  |  |  |  | -0.8050 | -0.9357 |  |  |  |
| Valeraldehyde |  |  | 1.6827 |  |  | 0.4606 | 0.1998 | -0.0308 |  |  |  |  |  |
| Valerophenone | 0.1872 | -0.1563 | -0.3434 | 1.2845 | 0.9115 | 0.5938 | 0.3256 | 0.0918 | -0.2428 | -0.4187 | -0.5940 | -0.7510 | -0.8670 |
| Vanillin | 0.3838 | 0.0347 | -0.1981 | -0.7119 | -0.9522 |  |  |  | -0.1312 | -0.3162 | -0.4860 | -0.6520 | -0.7890 |
| Vinylpentamethyldisiloxane | |  |  | -0.5352 | -0.8092 |  |  |  |  |  |  |  |  |

Table S-9

Retention factor database for HP-INNOWAX (60 – 220 °C)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | log60 | log80 | log100 | log120 | log140 | log160 | log180 | log200 | log220 |
| 1-Acetonaphthone |  |  |  |  |  |  | 1.3199 | 1.0257 | 0.7620 |
| 1-Bromododecane |  |  |  |  |  | 0.5722 | 0.3002 | 0.0805 | -0.1322 |
| 1-Bromonaphthalene |  |  |  |  |  | 1.2340 | 0.9455 | 0.6932 | 0.4594 |
| 1-Chloronaphthalene |  |  |  |  |  | 0.9866 | 0.7175 | 0.4839 | 0.2586 |
| 1-Hexyne | -0.2030 | -0.4647 | -0.6940 | -0.9031 | -1.0870 |  |  |  |  |
| 1-Naphthol |  |  |  |  |  |  |  |  | 1.2349 |
| 1-Nitronaphthalene |  |  |  |  |  |  | 1.4350 | 1.1385 | 0.8700 |
| 1,12-dodecanediol |  |  |  |  |  |  |  | 1.3949 | 1.0625 |
| 1,2-Dichlorobenzene |  | 1.3424 | 0.9875 | 0.6779 | 0.4072 | 0.1416 | -0.0655 | -0.2631 | -0.4136 |
| 1,2-Dimethylbenzene | 0.9104 | 0.5791 | 0.2905 | 0.0384 | -0.1824 | -0.4004 | -0.5699 | -0.7147 | -0.8505 |
| 1,2,4,5-Tetrachlorobenzene |  |  |  |  |  |  |  | 0.1677 |  |
| 1,2,4-Trichlorobenzene |  |  |  | 0.9814 | 0.6838 |  |  |  |  |
| 1,3-Dichlorobenzene |  | 1.1626 | 0.8216 | 0.5241 | 0.2640 |  |  |  |  |
| 1,3-Dimethylbenzene |  |  |  |  |  | -0.5184 | -0.6568 | -0.7966 | -0.8017 |
| 1,3-Dinitrobenzene |  |  |  |  |  |  | 1.3172 | 1.0220 | 0.7573 |
| 1,3,5-Triethylbenzene |  |  |  |  |  | 0.0254 | -0.1905 | -0.3779 | -0.5563 |
| 1,4-Dimethylbenzene | 0.7644 | 0.4444 | 0.1662 | -0.0787 | -0.2908 | -0.5059 | -0.6676 | -0.7979 | -0.9339 |
| 13-Dichloro-1,1,3,3-tetramethyldisiloxane | 0.0031 | -0.3570 |  |  | -0.9920 |  |  |  |  |
| 2-(1-naphthyl)ethanol |  |  |  |  |  |  |  |  | 1.1465 |
| 2-Acetonaphthone |  |  |  |  |  |  | 1.3957 | 1.0970 | 0.8265 |
| 2-Ethoxyethanol | 1.0103 | 0.6464 | 0.3306 | 0.0532 | -0.1895 |  |  |  |  |
| 2-Hexanone | 0.5968 | 0.2790 | 0.0024 | -0.2395 | -0.4515 |  |  |  |  |
| 2-Methoxycinnamaldehyde |  |  |  |  |  |  | 1.2715 | 0.9657 | 0.6986 |
| 2-Methoxyethanol | 0.8777 | 0.5305 | 0.2281 | -0.0369 | -0.2690 |  |  |  |  |
| 2-Methoxynaphthalene |  |  |  |  |  | 1.2333 | 0.9296 | 0.6731 | 0.3848 |
| 2-Methyl-2-butanol | 0.3580 | 0.0328 | -0.2483 | -0.4936 | -0.7094 |  |  |  |  |
| 2-Methylaniline |  |  |  |  |  | 0.6294 | 0.3652 | 0.1361 | -0.0721 |
| 2-Methylbutanol | 0.9723 | 0.5935 | 0.2655 | -0.0218 | -0.2711 |  |  |  |  |
| 2-Methylnaphthalene |  |  |  |  |  | 0.7352 | 0.4812 | 0.2601 | 0.0426 |
| 2-Methylphenol |  |  |  |  |  | 0.9303 | 0.6286 | 0.3624 | 0.1226 |
| 2-Methylpropanol | 0.6063 | 0.2600 | -0.0409 | -0.3010 | -0.5294 |  |  |  |  |
| 2-Naphthol |  |  |  |  |  |  |  |  | 1.3024 |
| 2-Nitroaniline |  |  |  |  |  |  | 1.5092 | 1.1906 | 0.9052 |
| 2-Nitrophenol |  |  |  |  |  | 0.6662 | 0.4154 | 0.2021 | 0.0034 |
| 2-Pentanone | 0.2816 | -0.0064 | -0.2570 | -0.4759 | -0.6756 |  |  |  |  |
| 2-Phenylethanol |  |  |  |  |  | 0.7922 | 0.5130 | 0.2788 | 0.0436 |
| 3-Methylaniline |  |  |  |  |  | 0.6939 | 0.4249 | 0.1892 | -0.0260 |
| 3-Methylbutanol | 0.9741 | 0.5951 | 0.2668 | -0.0205 | -0.2690 |  |  |  |  |
| 3-Methylphenol |  |  |  |  |  | 1.0823 | 0.7430 | 0.4860 | 0.2417 |
| 3-Nitroaniline |  |  |  |  |  |  |  |  | 1.2128 |
| 3,4-Dichloroanilne |  |  |  |  |  |  |  | 1.1913 | 0.8976 |
| 3,5-Dimethylphenol |  |  |  |  |  | 1.2210 | 0.8901 | 0.6010 | 0.3478 |
| 4-Chloroaniline |  |  |  |  |  | 1.2255 | 0.9041 | 0.6335 | 0.3885 |
| 4-Fluoroaniline |  |  |  |  |  |  |  | 0.1534 |  |
| 4-Methoxybenzyl alcohol |  |  |  |  |  |  | 1.0433 | 0.7478 | 0.4853 |
| 4-Methylphenol |  |  |  |  |  | 1.0680 | 0.7522 | 0.4740 | 0.2311 |
| 4-Nitrotoluene |  |  |  |  |  | 0.7668 | 0.5140 | 0.2900 | 0.0830 |
| Acenaphthene |  |  |  |  |  | 1.2439 | 0.9537 | 0.6979 | 0.4659 |
| Acenaphthylene |  |  |  |  |  | 1.2433 | 0.9537 | 0.6979 | 0.4659 |
| Acetophenone |  |  |  | 0.9986 | 0.6955 | 0.3991 | 0.1658 | -0.0405 | -0.2259 |
| alpha-Pinene |  |  | -0.1163 | -0.3265 | -0.5150 | -0.7102 | -0.8693 | -0.9612 | -1.0943 |
| Amyl cinnamal |  |  |  |  |  | 1.3399 | 1.0128 | 0.7173 | 0.4713 |
| Aniline |  |  |  |  | 0.8660 | 0.5383 | 0.2843 | 0.0533 | -0.1425 |
| Anisole |  |  |  |  |  | -0.1361 | -0.3307 | -0.5106 | -0.6624 |
| Anthracene |  |  |  |  |  |  |  | 1.3155 | 1.0401 |
| Benzaldehyde |  |  | 1.0654 | 0.7459 | 0.4663 | 0.1949 | -0.0181 | -0.2092 | -0.3759 |
| Benzamide |  |  |  |  |  |  |  | 1.2773 | 0.9796 |
| Benzene | 0.1822 | -0.0848 | -0.3134 | -0.5166 | -0.6979 |  |  |  |  |
| Benzophenone |  |  |  |  |  |  | 1.3239 | 1.0287 | 0.7624 |
| Benzyl 2-ethylhexyl phthalate |  |  |  |  |  |  |  | 1.9885 | 1.6431 |
| Benzyl alcohol |  |  |  |  |  | 0.7311 | 0.4541 | 0.2094 |  |
| beta-Pinene |  |  | 0.1085 | -0.1197 | -0.3216 | -0.5295 | -0.6951 |  | -0.9398 |
| Borneol |  |  |  | 1.0848 | 0.7580 | 0.4471 | 0.1979 | -0.0146 | -0.2027 |
| Butan-1-ol | 0.7793 | 0.4172 | 0.1037 | -0.1697 | -0.4084 |  |  |  |  |
| Butyl acetate | 0.5702 | 0.2445 | -0.0369 | -0.2823 | -0.4959 |  |  |  |  |
| Butyl benzyl phthalate |  |  |  |  |  |  |  |  | 1.8003 |
| Butyl cyclohexyl phthalate |  |  |  |  |  |  |  | 1.7561 | 1.3918 |
| Butyl decyl phthalate |  |  |  |  |  |  | 1.6862 | 1.3132 | 0.9801 |
| Butyl 2-ethylhexyl phthalate |  |  |  |  |  |  |  | 1.8443 | 1.5037 |
| Butyl octyl phthalate |  |  |  |  |  |  |  | 1.4179 |  |
| Butyl oleate |  |  |  |  |  |  | 1.5465 | 1.2157 | 0.8963 |
| Butyl stearate |  |  |  |  |  |  | 1.4141 |  | 0.7138 |
| Camphor |  |  |  |  |  | 0.2102 | 0.0003 | -0.1792 | -0.3462 |
| Carbon tetrachloride | -0.0228 | -0.2813 | -0.5022 | -0.6738 | -0.8884 |  |  |  |  |
| Carvone |  |  |  | 1.1575 | 0.8382 | 0.5328 | 0.2864 | 0.0757 | -0.1194 |
| Chlorobenzene | 0.9951 | 0.6541 | 0.3581 | 0.0988 | -0.1270 |  |  |  |  |
| Chloroform | 0.4042 | 0.0093 | -0.1749 | -0.4075 | -0.6102 |  |  |  |  |
| Cholestane |  |  |  |  |  |  |  |  | 1.3545 |
| Cinnamyl alcohol |  |  |  |  |  | 1.3895 | 1.0524 | 0.7548 | 0.4984 |
| Citronellal |  |  | 0.9618 | 0.6262 | 0.3358 | 0.0526 | -0.1736 | -0.3588 | -0.5338 |
| Coumarin |  |  |  |  |  |  | 1.2854 | 1.0032 | 0.7472 |
| Cyclohexanol |  | 1.1385 | 0.7730 | 0.4578 | 0.1825 |  |  |  |  |
| Cyclohexanone oxime |  |  |  |  |  | 0.6344 | 0.3668 | 0.1329 | -0.0769 |
| Decan-1-ol |  |  |  |  |  | 0.4956 | 0.2433 | -0.0169 | -0.2368 |
| Decane | 0.3196 | 0.0161 | -0.2483 | -0.4795 | -0.6810 |  |  |  |  |
| Di-(2-Methoxyethyl) phthalate | |  |  |  |  |  |  | 1.6985 | 1.3383 |
| Di-2-ethylhexyl phthalate |  |  |  |  |  |  |  | 1.8280 | 1.4873 |
| Di-n-Butyl phthalate |  |  |  |  |  |  | 1.6241 | 1.2807 | 0.9667 |
| Di-n-Butyl succinate |  |  |  |  |  | 1.0583 | 0.6262 | 0.3732 | 0.1437 |
| Di-n-Octyl phthalate |  |  |  |  |  |  |  |  | 1.7130 |
| Di(2-Ethoxyethyl) phthalate |  |  |  |  |  |  |  | 1.6807 | 1.3047 |
| Di(2-n-butoxyethyl) phthalate |  |  |  |  |  |  |  |  | 1.6770 |
| Dibenzofuran |  |  |  |  |  | 1.3403 | 1.0388 | 0.7739 | 0.5350 |
| Dibenzyl ether |  |  |  |  |  | 1.5179 | 1.1853 | 0.8930 | 0.6268 |
| Dibenzylamine |  |  |  |  |  |  | 1.3486 | 1.0450 | 0.7738 |
| Dicyclohexyl phthalate |  |  |  |  |  |  |  |  | 1.7872 |
| Dicyclohexylamine |  |  |  |  |  | 0.3788 | 0.1507 | -0.0527 | -0.2390 |
| Dicylcohexyl adipate |  |  |  |  |  |  |  | 1.6040 | 1.2765 |
| Diethyl diethylmalonate |  |  |  |  |  |  |  | -0.2014 | -0.3698 |
| Diethyl phthalate |  |  |  |  |  | 1.5632 | 1.2458 | 0.8625 | 0.5970 |
| Diethyl sebecate |  |  |  |  |  | 1.5021 | 1.1297 | 0.7633 | 0.4921 |
| Diisobutyl phthalate |  |  |  |  |  |  | 1.4102 | 1.0810 | 0.7834 |
| Dimethyl phthalate |  |  |  |  |  | 1.4528 | 1.1280 | 0.7773 | 0.5245 |
| Dioxane | 0.5441 | 0.2416 | -0.0200 | -0.2499 | -0.4515 |  |  |  |  |
| Diphenyl ether |  |  |  |  |  | 0.9685 | 0.6866 | 0.4387 | 0.2147 |
| Diphenylamine |  |  |  |  |  |  | 1.5035 | 1.1750 | 0.8802 |
| Dodecane | 0.9360 | 0.5696 | 0.2520 | -0.0255 | -0.2690 |  |  |  |  |
| Ethyl acetate | -0.0119 | -0.2837 | -0.5221 | -0.7333 | -0.8974 |  |  |  |  |
| Ethyl oleate |  |  |  |  |  |  |  | 0.9764 | 0.6251 |
| Ethylbenzene | 0.7416 | 0.4225 | 0.1467 | -0.0960 | -0.3068 |  |  |  |  |
| Eugenol |  |  |  |  |  | 1.2017 | 0.8803 | 0.5997 | 0.3522 |
| Geranial |  |  |  |  |  | 0.4950 | 0.2373 | 0.0166 | -0.1851 |
| Geraniol |  |  |  |  |  | 0.6501 | 0.3596 | 0.1120 | -0.1136 |
| Glycidoxypropyltrimethoxysilane | |  |  |  |  | 0.9541 | 0.6366 | 0.3584 | 0.1114 |
| Heptanal | 0.9187 | 0.5696 | 0.2668 | 0.0024 | -0.2284 |  |  |  |  |
| Heptane | -0.6403 | -0.8653 | -1.0329 |  |  |  |  |  |  |
| Hexachlorobenzene |  |  |  |  |  | 1.3176 | 1.0246 | 0.7660 | 0.5195 |
| Hexadecane |  |  |  | 0.8426 | 0.5258 | 0.1895 | -0.0591 | -0.2696 | -0.4667 |
| Hexamethylcyclotrisiloxane | -0.2886 | -0.5928 | -0.8263 |  | -1.2327 |  |  |  |  |
| Hexamethyldisiloxane | -0.9408 | -1.2316 |  |  |  |  |  |  |  |
| Hexanal | 0.6037 | 0.2863 | 0.0120 | -0.2274 | -0.4356 |  |  |  |  |
| Hexanol | 1.3965 | 0.9802 | 0.6193 | 0.3055 | 0.0271 |  |  |  |  |
| Hydroxycitronellal |  |  |  |  | 1.5856 |  |  | 0.5198 | 0.2611 |
| Iodobenzene |  |  |  |  |  | 0.2031 | -0.0052 | -0.1885 | -0.3521 |
| Isocyanatopropyltriethoxysilane | |  |  |  |  | 0.3038 | 0.0375 | -0.1949 | -0.4027 |
| Lilial |  |  |  |  |  | 1.0082 | 0.7113 | 0.4521 | 0.2207 |
| Limonene |  |  | 0.3116 | 0.0522 | -0.1715 | -0.4006 | -0.5808 | -0.7095 | -0.8580 |
| Linalool |  |  | 1.1125 | 0.7382 | 0.4173 |  | -0.1344 | -0.3359 | -0.5284 |
| Methacryloxypropyltrimethoxysilane | |  |  |  |  | 0.6894 | 0.3907 | 0.1304 | -0.1030 |
| Methyl abietate |  |  |  |  |  |  |  |  | 1.3824 |
| Methyl decanoate |  |  |  | 0.8679 | 0.5491 |  |  |  |  |
| Methyl eugenol |  |  |  |  | 1.3252 | 0.9489 | 0.6407 | 0.3746 | 0.1369 |
| Methyl hexanoate | 0.9224 | 0.5645 | 0.2541 | -0.0168 | -0.2523 |  |  |  |  |
| Methyl nonanoate |  |  | 0.9826 | 0.6404 | 0.3430 |  |  |  |  |
| Methyl octanoate |  | 1.1042 | 0.7404 | 0.4232 | 0.1456 |  |  |  |  |
| Naphthalene |  |  |  |  |  | 0.5608 | 0.3274 | 0.1137 | -0.0723 |
| Neral |  |  |  |  |  | 0.4165 | 0.1676 | -0.0449 | -0.2405 |
| Nicotine |  |  |  |  |  |  |  | 0.3609 |  |
| Nitrobenzene |  |  |  |  | 0.8610 |  |  |  |  |
| Nonanal |  | 1.1216 | 0.7651 | 0.4541 | 0.1818 |  |  |  |  |
| Nonane | -0.0053 | -0.2671 | -0.5261 | -0.7734 | -0.9659 |  |  |  |  |
| Octadecane |  |  |  |  |  | 0.5351 | 0.2551 | 0.0119 | -0.2068 |
| Octaethylcyclotetrasiloxane |  |  |  |  |  | 0.1308 | -0.1221 | -0.3439 | -0.5457 |
| Octan-1-ol |  |  | 1.1407 | 0.7728 | 0.4524 |  |  |  |  |
| Octan-2-ol |  |  |  |  |  |  |  | -0.5404 |  |
| Octanal | 1.2275 | 0.8467 | 0.5201 | 0.2321 | -0.0187 |  |  |  |  |
| Octane | -0.3116 | -0.5543 | -0.7591 | -0.9531 | -1.1162 |  |  |  |  |
| Octanophenone |  |  |  |  |  | 1.2957 | 0.9748 | 0.6920 | 0.4353 |
| Pentan-1-ol | 1.1073 | 0.7151 | 0.3754 | 0.0786 | -0.1807 |  |  |  |  |
| Pentan-2-ol | 0.6767 | 0.3420 | 0.0329 | -0.2354 | -0.4681 |  |  |  |  |
| Pentan-3-ol | 0.6598 | 0.3084 | 0.0036 | -0.2627 | -0.4923 |  |  |  |  |
| Phenanthrene |  |  |  |  |  |  |  | 1.3051 | 1.0350 |
| Phenol |  |  |  |  |  | 0.9447 | 0.6400 | 0.3719 | 0.1337 |
| Phenylacetate |  |  |  |  |  | 0.3185 | 0.0801 | -0.1282 | -0.2387 |
| Phenylcyclohexane |  |  |  |  |  | 0.4429 | 0.2105 | -0.0054 | -0.1775 |
| Phthalonitrile |  |  |  |  |  |  | 1.2689 | 0.9791 | 0.7252 |
| Propyl acetate | 0.2656 | -0.0314 | -0.2890 | -0.5128 | -0.7094 |  |  |  |  |
| Pyridine | 0.8895 | 0.5576 | 0.2707 | 0.0196 | -0.1984 |  |  |  |  |
| Quinoline |  |  |  |  |  | 0.8607 | 0.6008 | 0.3710 | 0.1599 |
| Styrene | 1.1254 | 0.7667 | 0.4542 | 0.1816 | -0.0562 |  |  |  |  |
| Terpinen-4-ol |  |  | 1.2424 | 0.8836 | 0.5452 | 0.2703 | 0.0416 | -0.1582 | -0.3396 |
| Tetrahydofuran | -0.0694 | -0.3087 | -0.5180 | -0.6908 | -0.8884 |  |  |  |  |
| Toluene | 0.4858 | 0.1910 | -0.0643 | -0.2871 | -0.4852 |  |  |  |  |
| Trans Stilbene |  |  |  |  |  |  | 1.3588 | 1.0504 | 0.7810 |
| Tri-n-Butyrin |  |  |  |  |  |  | 1.2672 | 0.9303 | 0.6279 |
| Tridecane | 1.2394 | 0.8393 | 0.4947 | 0.1938 | -0.0681 |  |  |  |  |
| Triethylamine | -0.4173 | -0.6500 | -0.8525 | -1.0474 | -1.2169 |  |  |  |  |
| Triphenylamine |  |  |  |  |  |  |  | 1.4698 | 1.1648 |
| Triphenylmethane |  |  |  |  |  |  |  | 1.4487 | 1.1404 |
| Undecane | 0.6265 | 0.2934 | 0.0036 | -0.2499 | -0.4714 | -0.6861 |  | -0.9919 | -1.1425 |
| Valeraldehyde | 0.2871 | 0.0000 | -0.2485 | -0.4655 | -0.6596 |  |  |  |  |
| Valerophenone |  |  |  |  |  | 0.7885 | 0.5152 | 0.2759 | 0.0588 |
| Vanillin |  |  |  |  |  |  |  | 1.0766 |  |